Tables of Molecular Vibrational Frequencies

Part 6

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The compilations of fundamental vibrational frequencies of molecules previously published in the NSRDS-NBS publication series and in this journal are here extended to 55 additional molecules. Selected values of the fundamental vibrational frequencies are given for each molecule, together with observed infrared and Raman spectral data and citations to the original literature. The selection of vibrational fundamentals has been based on careful studies of the spectral data and comprehensive normal-coordinate analyses. An estimate of the accuracy of the selected values is included. The tables provide a convenient source of information for those who require vibrational energy levels and related properties in molecular spectroscopy, thermodynamics, analytical chemistry, and other fields of physics and chemistry.

Key words: Fundamental frequencies; infrared spectra; polyatomic molecules; Raman spectra; vibrational frequencies.

1. Introduction

Establishing the assignment of molecular vibrational frequencies has fundamental importance in elucidating various problems in physics and chemistry. The information concerning the force field and motion of atoms in a molecule can be most directly derived from its vibrational frequencies. If all the vibrational frequencies of a molecule are known, as well as the molecular structure, thermodynamic quantities can be easily computed on the ideal gas model. Thus, the need for a tabulation of evaluated reference data on molecular vibrational frequencies has often been felt by many investigators. In 1964 a project for producing such tables was initiated at the University of Tokyo in cooperation with the National Standard Reference Data System of the National Bureau of Standards. The evaluated data resulting from this project were first published in the three parts of *Tables of Molecular Vibrational Frequencies* [1].[1] A *Consolidated Volume* [2] of these tables appeared in 1972 which includes revised versions of all the tables in ref. [1] plus tables for 52 additional molecules (a total of 223 molecules). A fifth set of tables, covering 58 molecules, was published in Volume 1 of this journal [3].

2. Molecules Selected

The present volume contains tables of fundamental vibrational frequencies for 55 additional molecules. The molecules were selected from basic organic and inorganic molecules for which the vibrational assignments have been established with little ambiguity. The effort of extending the tables to many other important molecules is continuing in this laboratory. Diatomic molecules and electronically excited species are not included in this volume, since refs. [4], [5], and [6] contain good compilations of data for them.

Rotational isomers are treated as independent molecular species, and a separate table is made for each of the isomers. When the gas and liquid state spectra are significantly different from each other, they are tabulated separately.

A list of the molecules covered here is given at the beginning of the tables. The molecules are numbered starting with number 282, continuing the designations of Part 5 of the tables. In sum, these tables now offer data on nearly 340 molecules. To assist the reader in finding the information he needs, two indices are appended, covering the contents of the Consolidated Volume, plus Part 5 and the present material. The first index is ordered by structural and symmetry factors, and the second by empirical formula.

3. Description of Tables

3.1. Symmetry

The symmetry (point group) of each molecule is given by the Schoenflies notation. Detailed discussions of symmetry properties will be found in refs. [7] and [8].

3.2. Symmetry Number

The symmetry number, σ, is used in the calculation of thermodynamic quantities. It is the number of indistinguishable positions into which the molecule can be transformed by simple rigid rotations. A general discussion and pertinent formulas may be found in ref. [8], page 508.

3.3. Symmetry Species

In the table, the normal modes are divided into the symmetry species of the point group to which the molecule belongs. The ordering of species in each point group is given in table I, which is a summary of tables

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[1] Figures in brackets indicate literature references in section 5.

12–30 of ref. [8]. When a molecule has two or three planes of symmetry, the relationship between the vibrational modes and symmetry species cannot be defined uniquely. In such cases we generally follow the notation adopted in ref. [8].

3.4. Numbering of Frequencies

The numbering is indicated by ν_i given in the second column of each table. The normal modes are first grouped into symmetry species, and then those in each species are ordered from higher to lower values of the frequency. However, we always denote the bending vibration of a linear triatomic molecule as ν_2, following the widely accepted tradition. For some deuterated compounds the frequencies are arranged so that the same ν_i numbering is given to the corresponding vibrational modes of deuterated and normal compounds.

TABLE I. Ordering of symmetry species

(In the present article small letters are used to designate the species of fundamental frequencies)

Point group	Symmetry species
C_2	A, B
C_s	A', A''
C_i	A_g, A_u
C_{2v}	A_1, A_2, B_1, B_2
C_{2h}	A_g, A_u, B_g, B_u
D_2	A, B_1, B_2, B_3
D_{2h}	$A_g, A_u, B_{1g}, B_{1u}, B_{2g}, B_{2u}, B_{3g}, B_{3u}$
C_{3v}	A_1, A_2, E
D_3	A_1, A_2, E
C_{5v}	A_1, A_2, E_1, E_2
$C_{\infty v}$	$\Sigma^+, \Sigma^-, \pi, \Delta, \Phi, \ldots$
C_{4v}, D_4, D_{2d}	A_1, A_2, B_1, B_2, E
C_{6v}, D_6	$A_1, A_2, B_1, B_2, E_1, E_2$
D_{3d}	$A_{1g}, A_{1u}, A_{2g}, A_{2u}, E_g, E_u$
D_{4d}	$A_1, A_2, B_1, B_2, E_1, E_2, E_3$
D_{3h}	$A_1', A_1'', A_2', A_2'', E', E''$
D_{5h}	$A_1', A_1'', A_2', A_2'', E_1', E_1'', E_2', E_2''$
D_{4h}	$A_{1g}, A_{1u}, A_{2g}, A_{2u}, B_{1g}, B_{1u}, B_{2g}, B_{2u}, E_g, E_u$
D_{6h}	$A_{1g}, A_{1u}, A_{2g}, A_{2u}, B_{1g}, B_{1u}, B_{2g}, B_{2u}, E_{1g}, E_{1u}\ E_{2g}, E_{2u}$
$D_{\infty h}$	$\Sigma_g^+, \Sigma_u^+, \Sigma_g^-, \Sigma_u^-, \pi_g, \pi_u, \Delta_g, \Delta_u, \Phi_g, \Phi_u, \ldots$
C_3	A, E
C_6	A, B, E_1, E_2
S_6	A_g, A_u, E_g, E_u
C_{3h}	A', A'', E', E''
C_{4h}	$A_g, A_u, B_g, B_u, E_g, E_u$
C_{6h}	$A_g, A_u, B_g, B_u, E_{1g}, E_{1u}, E_{2g}, E_{2u}$
T_d, O	A_1, A_2, E, F_1, F_2
O_h	$A_{1g}, A_{1u}, A_{2g}, A_{2u}, E_g, E_u, F_{1g}, F_{1u}, F_{2g}, F_{2u}$
T	A, E, F

3.5. Approximate Type of Mode

The approximate type of mode given in the third column of each table is the local symmetry coordinate which makes the maximum contribution to the normal mode. Local symmetry coordinates are defined for several chemical groups in table II. It should be emphasized that two or more local symmetry coordinates are often coupled strongly in a normal coordinate, and the approximate type of mode given in the table has only limited significance in such a case.

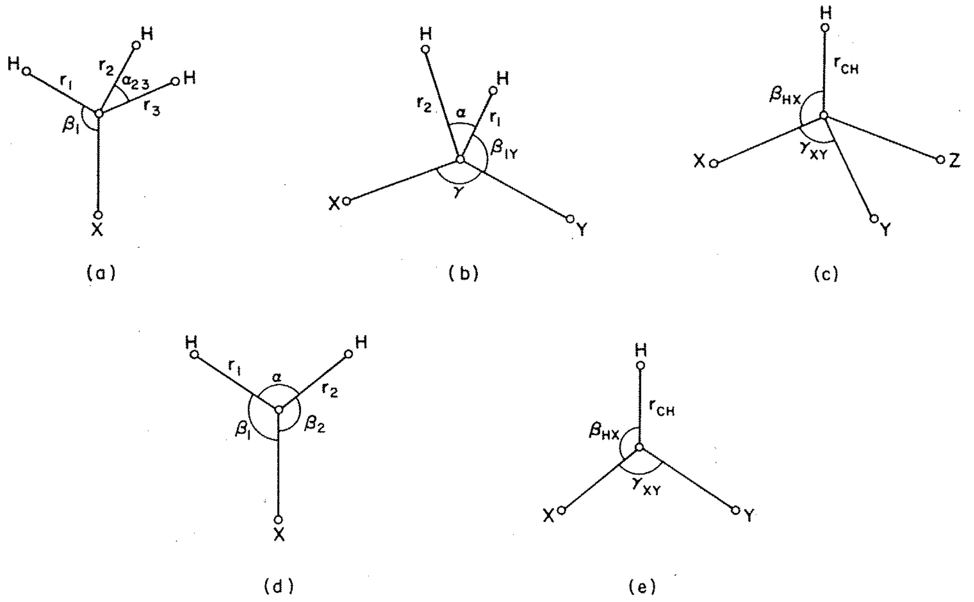
The following abbreviations are used for the type of mode:

stretch.	stretching
deform.	deformation
rock.	rocking
twist.	twisting
wag.	wagging
scis.	scissors
bend.	bending
sym. or s-	symmetrical
anti. or a-	antisymmetrical
deg. or d-	degenerate
ip-	in-plane
op-	out-of-plane

TABLE II. Definition of local symmetry coordinates

(a) Local symmetry coordinates for the CH_3 group (see fig. 1a)
CH_3 symmetrical stretching: $(\Delta r_1+\Delta r_2+\Delta r_3)\ /\ \sqrt{3}$
CH_3 degenerate stretching: $(2\Delta r_1-\Delta r_2-\Delta r_3)\ /\ \sqrt{6}$
$(\Delta r_2-\Delta r_3)\ /\ \sqrt{2}$
CH_3 symmetrical deformation:
$(\Delta\alpha_{23}+\Delta\alpha_{31}+\Delta\alpha_{12}-\Delta\beta_1-\Delta\beta_2-\Delta\beta_3)\ /\ \sqrt{6}$
CH_3 degenerate deformation: $(2\Delta\alpha_{23}-\Delta\alpha_{31}-\Delta\alpha_{12})\ /\ \sqrt{6}$
$(\Delta\alpha_{31}-\Delta\alpha_{12})\ /\ \sqrt{2}$
CH_3 rocking: $(2\Delta\beta_1-\Delta\beta_2-\Delta\beta_3)\ /\ \sqrt{6}$
$(\Delta\beta_2-\Delta\beta_3)\ /\ \sqrt{2}$.
(b) Local symmetry coordinates for the CH_2 group (see fig. 1b)
CH_2 symmetrical stretching: $(\Delta r_1+\Delta r_2)\ /\ \sqrt{2}$
antisymmetrical stretching: $(\Delta r_1-\Delta r_2)\ /\ \sqrt{2}$
CH_2 scissors: $(4\Delta\alpha-\Delta\beta_{1X}-\Delta\beta_{2X}-\Delta\beta_{1Y})\ /\ \sqrt{20}$
CH_2 wagging: $(\Delta\beta_{1X}+\Delta\beta_{2X}-\Delta\beta_{1Y}-\Delta\beta_{2Y})\ /\ 2$
CH_2 twisting: $(\Delta\beta_{1X}-\Delta\beta_{2X}-\Delta\beta_{1Y}+\Delta\beta_{2Y})\ /\ 2$
CH_2 rocking: $(\Delta\beta_{1X}-\Delta\beta_{2X}+\Delta\beta_{1Y}-\Delta\beta_{2Y})\ /2.\ 2.$
(c) Local symmetry coordinates for the CH group (see fig. 1c)
CH stretching: Δr_{CH}
CH bending: $(2\Delta\beta_{HX}-\Delta\beta_{HY}-\Delta\beta_{HZ})\ /\ \sqrt{6}$
$(\Delta\beta_{HY}-\Delta\beta_{HZ})\ /\ \sqrt{2}$
(d) Local symmetry coordinates for the planar CH_2 group (see fig. 1d)
CH_2 symmetrical stretching: $(\Delta r_1+\Delta r_2)\ /\ \sqrt{2}$
CH_2 antisymmetrical stretching: $(\Delta r_1-\Delta r_2)\ /\ \sqrt{2}$
CH_2 scissors: $(2\Delta\alpha-\Delta\beta_1-\Delta\beta_2)\ /\ \sqrt{6}$
CH_2 rocking: $(\Delta\beta_1-\Delta\beta_2)\ /\ \sqrt{2}$
CH_2 wagging: $\Delta\theta\cdot\sin\alpha$.
(e) Local symmetry coordinates for the planar CH group (see fig. 1e)
CH stretching: Δr_{CH}
in-plane CH bending: $(\Delta\beta_{HX}-\Delta\beta_{HY})\ /\ \sqrt{2}$
out-of-plane CH bending: $\Delta\theta_H\cdot\sin\gamma_{XY}$.

The plane to which the in-plane and out-of-plane expressions refer is the molecular plane of a planar molecule or the symmetry plane of a general molecule belonging to point group C_s. Local symmetry coordinates of the CX_3 groups attached to a relatively large molecule are designated as s-stretch., s-deform., d-stretch., and d-deform. In such a molecule with low



(a) (b) (c)

(d) (e)

FIGURE 1. Parameters of methyl, methylene, and methin groups.

TABLE III. Uncertainty code for the selected values of frequencies

Notation	Uncertainty	Basis*
	cm^{-1}	
A	$0 \sim 1$	(i) Gas, grating spectrometer, rotational fine structure accurately analyzed. (ii) Gas, grating spectrometer, a sharp Q branch.
B	$1 \sim 3$	(i) Gas, grating spectrometer, rotational fine structure partly analyzed. (ii) Gas, prism spectrometer, fairly high resolution (e.g., $700 \sim 1000$ cm^{-1} for NaCl prism).
C	$3 \sim 6$	(i) Gas, prism spectrometer, low resolution (e.g., $1000 \sim 2000$ cm^{-1} for NaCl prism). (ii) Solid, liquid or solution, accurate measurement.
D	$6 \sim 15$	(i) Gas, prism spectrometer, very low resolution (e.g., > 2000 cm^{-1} for NaCl prism). (ii) Solid, liquid or solution, inaccurate measurement.
E	$15 \sim 30$	(i) Value estimated from Fermi resonance doublet. (ii) Value estimated from overtone or combination tone. (iii) Calculated frequency.

*The uncertainty assigned here to each method of measurement is a typical value; greater accuracy is often achieved with some of the methods.

symmetry none of the normal vibrations are genuinely "symmetrical" or "degenerate" with respect to the three-fold symmetry axis of the CX_3 group. However, the notation is retained because it is convenient for indicating the correspondence between similar modes in large and small molecules.

3.6. Selected Value of Frequency

The fundamental frequency ν_i is defined as the difference between the term value $G(v_i = 1$, all other $v_j = 0)$ and $G(v_i = 0$, and other $v_j = 0)$ expressed in cm^{-1}. Fundamental frequencies rather than harmonic frequencies (ω_j) are listed in the table. Although harmonic frequencies are of greater physical significance, they are accurately known only for a small number of polyatomic molecules. The selected values are rounded to the nearest 1 cm^{-1}.

The letter code, A, B, C, D, or E following the selected value of frequency indicates the evaluator's judgment of the accuracy of the value. The basis for estimating accuracy of an observed frequency is given in table III, together with the range of uncertainty in cm^{-1} for each grade.

Frequencies derived from infrared and Raman measurements in the gaseous state are chosen unless otherwise mentioned. When a detailed analysis of the rotational fine structure of an infrared band is available, the band center ν_0 is chosen as the fundamental frequency and given the uncertainty code A (see below). For a well-analyzed perpendicular band of a symmetric top molecule, the frequency listed contains the nonvibrational part $A'\zeta^2$, where A' is the rotational constant of the vibrational level and ζ of the Coriolis coupling constant. This is in accord with the definition of ν_0 given in ref. [8], page 404 and equation (IV, 60).

When the spectra in the gaseous state are not available, the frequencies observed in the liquid or solid state are listed. When no spectral data have been obtained, the results of normal vibration calculations or of some other methods of estimating frequencies are listed with the grade D or E.

The torsional frequency may be calculated using the barrier height and reduced moment derived from microwave spectroscopy. The value obtained in this way is given as MW (frequency in cm^{-1}) in the "Comments" column or as a footnote for comparison with the value observed or calculated by the normal coordinate treatment. Microwave data are taken from ref. [10] unless otherwise noted.

For many molecules the assignments given in the literature have been checked by normal vibration calculations carried out in this laboratory as part of the project. Revisions in some assignments have been made as a result of these calculations. The details of the normal coordinate treatment and evaluation of force constants will be found in ref. [9].

Thermodynamic quantities may be computed in most cases by employing the harmonic oscillator partition function and by assuming that the harmonic frequencies are not much different from the fundamental frequencies given here. Such an approximation is not adequate, however, for molecules with highly anharmonic motions such as internal rotation, inversion, and ring-puckering. The vibrational partition function should be formed for these molecules by summing the terms due to the individual energy levels.

3.7. Infrared and Raman Spectra

The observed infrared and Raman frequencies are given in the fifth and sixth columns of each table. Rough estimates of relative intensities, band shapes, and polarization characteristics are also given. An additional significant figure is included here when warranted. The abbreviations used are as follows:

VS	very strong
S	strong
M	medium
W	weak
VW	very weak
ia	inactive
b	broad
vb	very broad
sh	shoulder
p	polarized
dp	depolarized

For some molecules the relative intensities of Raman lines are indicated by numbers from one to ten in accordance with the tradition widely used. These estimates of intensity are taken from the original references without any attempt at critical evaluation.

3.8. Comments

In the last column of each table brief comments are added to give special information which is not indicated in the preceding columns. The abbreviations used in this column are as follows:

FR	Fermi resonance with an overtone or a combination tone indicated in the parentheses.
OC	Frequency estimated from an overtone or a combination tone indicated in the parentheses.
CF	Calculated frequency.
SF	Calculation shows that frequency approximately equals that of the vibration indicated in the parentheses.
OV	Overlapped by the band indicated in the parentheses.
MW	Torsional frequency calculated from microwave spectroscopic data.

3.9. Footnotes and References

The footnote is used to supply other necessary information which cannot be placed simply in the column of Comments. The references accompanying the table are not comprehensive. Only the papers relevant to the present tabulation are cited. The abbreviations IR, R, MW, and Th stand for infrared, Raman, microwave, and theoretical, respectively.

4. Acknowledgements

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5. References

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6. List of Tables of Molecular Vibrational Frequencies

No. 282 Water $H_2{}^{18}O$

Symmetry C_{2v} **Symmetry number $\sigma = 2$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	*cm*$^{-1}$ (Gas)	*cm*$^{-1}$	
a_1	ν_1	Sym. stretch.	3650 A	3649.68		
	ν_2	Bend.	1588 A	1588.275		
b_1	ν_3	Anti. stretch.	3742 A	3741.58		

References

[1] IR. W. S. Benedict, Mem. Soc. Roy. Sci. Liege, **18**, 557 (1957).
[2] IR. P. E. Fraley, K. N. Rao, and L. H. Jones, J. Mol. Spectry. **29**, 312 (1969).
[3] IR. J. G. Williamson, K. N. Rao, and L. H. Jones, J. Mol. Spectry. **40**, 372 (1971).

No. 283 Sulfur dioxide $S^{18}O_2$

Symmetry C_{2v} **Symmetry number $\sigma = 2$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	*cm*$^{-1}$ (Gas)	*cm*$^{-1}$	
a_1	ν_1	Sym. stretch.	1101 B	1100.65		
	ν_2	Bend.	497 B	496.7		
b_1	ν_3	Anti. stretch.	1318 B	1317.9		

Reference

[1] IR. A. Barbe and P. Jauve, J. Mol. Spectry. **38**, 273 (1971).

No. 284 Hypochlorous acid HOCl

Symmetry C_s **Symmetry number $\sigma = 1$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	*cm*$^{-1}$ (Gas)	*cm*$^{-1}$	
a'	ν_1	OH stretch.	3609 A	3609 M		
	ν_2	OCl stretch.	739 C	739 M		
	ν_3	Bend.	1242 C	1242 S		

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[2] IR. R. A. Ashby, J. Mol. Spectry. **23**, 439 (1967).
[3] IR. I. Schwager and A. Arkell, J. Amer. Chem. Soc. **89**, 6006 (1967).

No. 285 Hypochlorous acid–d DOCl

Symmetry C_s **Symmetry number $\sigma = 1$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1}	
a'	ν_1	OD stretch.	2666 B	2666 M		
	ν_2	OCl stretch.	739 C	739 M		
	ν_3	Bend.	911 C	911 S		

References

See No. 284 (HOCl)

No. 286 Thionitrosyl–S–fluoride NSF

Symmetry C_s **Symmetry number $\sigma = 1$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1}	
a'	ν_1	NS stretch.	1372 C	1372 VS		
	ν_2	SF stretch.	640 C	640 VS		
	ν_3	Bend.	366 C	366 S		

Reference

[1] IR. H. Richert and O. Glemser, Z. Anorg. Allg. Chem. **307**, 328 (1961).

No. 287 Thionitrosyl–S–chloride NSCl

Symmetry C_s **Symmetry number $\sigma = 1$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1}	
a'	ν_1	NS stretch.	1325 C	1325		
	ν_2	SCl stretch.	414 C	414		
	ν_3	Bend.	273 D			OC($\nu_2+\nu_3$, $2\nu_3$).

Reference

[1] IR. A. Müller, G. Nagarajan, O. Glemser, S. F. Cyvin, and J. Wegener, Spectrochim. Acta **23A**, 2683 (1967).

No. 288 trans–1,2–Difluorodiazine N_2F_2

Symmetry C_{2h} **Symmetry number $\sigma = 2$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Gas)	
a_g	ν_1	NN stretch.	1523 C	ia	1523 (2)	
	ν_2	NF stretch.	1018 C	ia	1018 (5)	
	ν_3	FNN deform.	603 C	ia	603 (10)	
a_u	ν_4	Torsion	364 B	363.5 M	ia	
b_u	ν_5	NF stretch.	991 A	991.01 VS	ia	
	ν_6	FNN deform.	423 C	423 M	ia	

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[2] IR.R. S.–T. King and J. Overend, Spectrochim. Acta **22**, 689 (1966).
[3] IR. S.–T. King and J. Overend, Spectrochim. Acta **23A**, 2875 (1967).
[4] IR.R. J. Shamir and H. H. Hyman, Spectrochim. Acta, **23A**, 1191 (1967).

No. 289 Chlorine trifluoride ClF_3

Symmetry C_{2v} **Symmetry number $\sigma = 2$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Gas)	
a_1	ν_1	ClF stretch.	752 C	751 S	752.1 S, p	
	ν_2	ClF_2 s–stretch.	529 C	530 M	529.3 VS, p	
	ν_3	ClF_2 ip–deform.	328 C	328 S	337 W, p 321	OV(ν_6).
b_1	ν_4	ClF_2 a–stretch.	702 C	702 VS		
	ν_5	ClF_2 ip–deform.	442 C	442 W	431 W, dp	
b_2	ν_6	ClF_2 op–deform.	328 D	328 S		OV(ν_3).

Reference

[1] IR.R. H. Selig, H. H. Claassen, and J. H. Holloway, J. Chem. Phys. **52**, 3517 (1970).

No. 290 Bromine trifluoride BrF_3

Symmetry C_{2v} **Symmetry number $\sigma = 2$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Gas)	
a_1	ν_1	BrF stretch.	675 C	675 S	675 S, p	
	ν_2	BrF_2 s–stretch.	552 C	552 W	552 VS, p	
	ν_3	BrF_2 ip–deform.	242 C	242 S	233 W, p	OV(ν_6).
b_1	ν_4	BrF_2 a–stretch.	614 C	614 VS	612 VW	
	ν_5	BrF_2 ip–deform.	350 C	350 VW		
b_2	ν_6	BrF_2 op–deform.	242 D	242 S		OV(ν_3).

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[1] IR.R. H. Selig, H. H. Claassen, and J. H. Holloway, J. Chem. Phys. **52,** 3517 (1970).

[2] IR. K. O. Christe, E. C. Curtis, and D. Pilipovich, Spectrochim. Acta **27A,** 931 (1971).

No. 291 Ammonia–t_3 NT_3

Symmetry C_{3v} **Symmetry number $\sigma = 3$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	Sym. stretch.	2014 A	2014.1		
	ν_2	Sym. deform.	657 B	656.4 s[a] 657.2 a[a]		
e	ν_3	Deg. stretch.	2185 A	2184.8		
	ν_4	Deg. deform.	996 A	996.3		

[a] "s" and "a" refer to symmetric and antisymmetric levels [1].

References

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No. 292 Arsenic trifluoride AsF_3

Symmetry C_{3v} **Symmetry number $\sigma = 3$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1	ν_1	Sym. stretch.	741 A	740.5 S	707 (10)	
	ν_2	Sym. deform.	337 B	336.5 M	341 (2)	
e	ν_3	Deg. stretch.	702 B	702.2 S	644 (9)	
	ν_4	Deg. deform.	262 B	262.3 M	274 (4)	

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[3] IR.Th. I. W. Levin and S. Abramowitz, J. Chem. Phys. **44**, 2562 (1966).
[4] IR.Th. L. C. Hoskins, J. Chem. Phys. **45**, 4594 (1966).
[5] Th. A. M. Mirri, J. Chem. Phys. **47**, 2823 (1967).
[6] IR. S. Reichman and J. Overend, Spectrochim. Acta **26A**, 379 (1970).
[7] Th. S. Reichman, D. F. Smith, Jr. and J. Overend, Spectrochim. Acta **26A**, 927 (1970).

No. 293 Hydrogen persulfide H_2S_2

Symmetry C_2 **Symmetry number $\sigma = 2$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Liquid)	
a	ν_1	SH stretch.	2556 A	2555.78	2509 (2), dp	
	ν_2	SH bend.	883 D		883 (2), dp	
	ν_3	SS stretch.	509 D		509 (9)	
	ν_4	Torsion	416 B	416		
b	ν_5	SH stretch.	2559 A	2558.64		
	ν_6	SH bend.	886 C	886		

References
[1] IR. M. K. Wilson and R. M. Badger, J. Chem. Phys. **17**, 1232 (1949).
[2] R. F. Fehér, W. Laue, and G. Winkhaus, Z. Anorg. Allg. Chem. **288**, 113 (1956).
[3] IR. R. L. Redington, J. Mol. Spectry. **9**. 469 (1962).
[4] IR. B. P. Winnewisser, J. Mol. Spectry. **36**, 414 (1970).

No. 294 Difluoro disulphane F_2S_2

Symmetry C_2 **Symmetry number $\sigma = 2$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm⁻¹	cm⁻¹ (Gas)	cm⁻¹ (Liquid)	
a	ν_1	SF stretch.	717 B	717.0		
	ν_2	SS stretch.	615 B	614.6	623 p	
	ν_3	SF bend.	320 B	319.8	322 p	
	ν_4	Torsion	183 C	182.5	193 p	
b	ν_5	SF stretch.	681 B	680.8	683	
	ν_6	SF bend.	301 C	301	297 dp	

References

[1] IR. F. Seel and R. Budenz, Chem. Ber. **98,** 251 (1965).
[2] IR.R. R. D. Brown and G. P. Pez, Spectrochim. Acta **26A,** 1375 (1970).

No. 295 Difluoroamine NF_2H

Symmetry C_s **Symmetry number $\sigma = 1$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm⁻¹	cm⁻¹ (Gas)	cm⁻¹	
a′	ν_1	NH stretch.	3193 C	3193 W		
	ν_2	NH bend.	1307 B	1307 S		
	ν_3	NF_2 s-stretch.	972 B	972 S		
	ν_4	NF_2 scis.	500 C	500 M		
a″	ν_5	NH bend.	1424 B	1424 S		
	ν_6	NF_2 a-stretch.	888 C	888 VS		

Reference

[1] IR. J. J. Comeford, D. E. Mann, J. L. Schoen, and D. R. Lide, Jr., J. Chem. Phys. **38,** 461 (1963).

No. 296 Ruthenium tetroxide RuO_4

Symmetry T_d **Symmetry number $\sigma = 12$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm $^{-1}$	*cm* $^{-1}$ (Gas)	*cm* $^{-1}$ (Liquid)	
a_1	ν_1	Sym. stretch.	885 C	ia	885.3 S (Gas)	
e	ν_2	Deg. deform.	322 C	ia	322.4 M	
f_2	ν_3	Deg. stretch.	921 C	921.0	912.9 W	
	ν_4	Deg. deform.	336 C	336.0	333 W	

References

[1] IR.	R. E. Dodd, Trans. Faraday Soc. **55,** 1480 (1959).
[2] IR.	M. H. Ortner, J. Chem. Phys. **34,** 559 (1961).
[3] R.	G. Davidson, N. Logan, and A. Morris, Chem. Commun. **1968,** 1044.
[4] R.	W. P. Griffith, J. Chem. Soc. **A1968,** 1663.
[5] IR.	A. Müller and B. Krebs, J. Mol. Spectry. **26,** 136 (1968).
[6] IR.R.	I. W. Levin and S. Abramowitz, J. Chem. Phys. **50,** 4860 (1969).
[7] Th.	R. S. McDowell, J. Chem. Phys. **53,** 4407 (1970).
[8] IR.R.	R. S. McDowell, L. B. Aspery and L. C. Hoskins, J. Chem. Phys. **56,** 5712 (1972).

No. 297 Osmium tetroxide $Os^{16}O_4$

Symmetry T_d **Symmetry number $\sigma = 12$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm $^{-1}$	*cm* $^{-1}$ (Gas)	*cm* $^{-1}$ (Gas)	
a_1	ν_1	Sym. stretch.	965 B	ia	965.2	
e	ν_2	Deg. deform.	333 B	ia	333.1	
f_2	ν_3	Deg. stretch.	960 B	960.5	960.1	
	ν_4	Deg. deform.	329 B	329.0	322.7	

References

[1] IR.	N. J. Hawkins and W. W. Sabal, J. Chem. Phys. **25,** 775 (1956).
[2] IR.	R. E. Dodd, Trans. Faraday Soc. **55,** 1480 (1959).
[3] IR.	I. W. Levin and S. Abramowitz, Inorg. Chem. **5,** 2024 (1966).
[4] IR.	R. S. McDowell, Inorg. Chem. **6,** 1759 (1967).
[5] R.	W. P. Griffith, J. Chem. Soc. **A1968,** 1663.
[6] R.	G. Davidson, N. Logan, and A. Morris, Chem. Commun. **1968,** 1044.
[7] R.	I. W. Levin, Inorg. Chem. **8,** 1018 (1969).
[8] R.	J. L. Huston and H. H. Claassen, J. Chem. Phys. **52,** 5646 (1970).
[9] IR.	C. G. Barraclough and M. M. Sinclair, Spectrochim. Acta **26A,** 207 (1970).
[10] IR.R.	R. S. McDowell and M. Goldblatt, Inorg. Chem. **10,** 625 (1971).

No. 298 Osmium tetroxide $Os^{18}O_4$

Symmetry T_d **Symmetry number $\sigma = 12$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (CCl_4 soln.)	
a_1	ν_1	Sym. stretch.	910 C	ia	909.7	
e	ν_2	Deg. deform.	317 C	ia	316.6	
f_2	ν_3	Deg. stretch.	912 B	911.8		
	ν_4	Deg. deform.	313 B	312.7		

References

[1] IR.	C. G. Barraclough and M. M. Sinclair, Spectrochim. Acta **26A**, 207 (1970).
[2] IR.R.	R. S. McDowell and M. Goldblatt, Inorg. Chem. **10**, 625 (1971).

No. 299 Dichlorosilane SiH_2Cl_2

Symmetry C_{2v} **Symmetry number $\sigma = 2$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1	ν_1	SiH_2 s-stretch.	2224 C	2224 S	2221 S, p	
	ν_2	SiH_2 scis.	954 C	954 S	942 W, dp	
	ν_3	$SiCl_2$ s-stretch.	527 C	527 W	514 S, p	
	ν_4	$SiCl_2$ scis.	188 D		188 M, dp	
a_2	ν_5	SiH_2 twist.	710 D	ia	710 W, dp	
b_1	ν_6	SiH_2 a-stretch.	2237 B	2237 S		
	ν_7	SiH_2 rock.	602 C	602 W		
b_2	ν_8	SiH_2 wag.	876 B	876 VS	868 VW, dp	
	ν_9	$SiCl_2$ a-stretch.	590 C	590 S	566 VW, dp	

References

[1] IR.R.	J. A. Hawkins and M. K. Wilson, J. Chem. Phys. **21**, 360 (1953).
[2] IR.	J. A. Hawkins, S. R. Polo, and M. K. Wilson, J. Chem. Phys. **21**, 1122 (1953).
[3] IR.	D. H. Christensen and O. F. Nielsen, J. Mol. Spectry. **27**, 489 (1968).
[4] Th.	D. H. Christensen and O. F. Nielsen, J. Mol. Spectry. **33**, 425 (1970).

No. 300 Dichlorosilane–d_2 SiD_2Cl_2

Symmetry C_{2v} **Symmetry number $\sigma = 2$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	SiD_2 s–stretch.	1608 C	1608 S		
	ν_2	SiD_2 scis.	695 C	695 S		
	ν_3	$SiCl_2$ s–stretch.	519 C	519 W		
	ν_4	$SiCl_2$ scis.	187 D	187 W		
a_2	ν_5	SiD_2 twist.	506 D	ia		CF.
b_1	ν_6	SiD_2 a–stretch.	1637 C	1637 S		
	ν_7	SiD_2 rock.	466 B	466 W		
b_2	ν_8	SiD_2 wag.	663 B	663 VS		
	ν_9	$SiCl_2$ a–stretch.	566 C	566 W		

References

[1] IR. D. H. Christensen and O. F. Nielsen, J. Mol. Spectry. **27**, 489 (1968).

[2] Th. D. H. Christensen and O. F. Nielsen, J. Mol. Spectry. **33**, 425 (1970).

No. 301 Dibromosilane SiH_2Br_2

Symmetry C_{2v} **Symmetry number $\sigma = 2$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1	ν_1	SiH_2 s–stretch.	2206 D	2200 S	2206 S, p	
	ν_2	SiH_2 scis.	942 C	942 VS	925 W, dp	
	ν_3	$SiBr_2$ s–stretch.	407 C	407 M	393 S, p	
	ν_4	$SiBr_2$ scis.	122 D		122 M, p	
a_2	ν_5	SiH_2 twist.	688 D	ia	688 W, dp	
b_1	ν_6	SiH_2 a–stretch.	2232 D	2200 S	2232 W, dp	
	ν_7	SiH_2 rock.	556 C	556 S		
b_2	ν_8	SiH_2 wag.	843 C	843 VS	828 VW, dp	
	ν_9	$SiBr_2$ a–stretch.	471 C	471 S	456 W, dp	

References

[1] R. F. François and M. Buisset, Comptes Rendus **230**, 1946 (1950).

[2] IR. D. W. Mayo, H. E. Opitz, and J. S. Peake, J. Chem. Phys. **23**, 1344 (1955).

No. 302 Phosphoryl fluorodichloride $OPFCl_2$

Symmetry C_s **Symmetry number $\sigma = 1$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm $^{-1}$	*cm* $^{-1}$	*cm* $^{-1}$ (Liquid)	
a'	ν_1	PO stretch.	1331 D		1331 p	
	ν_2	PF stretch.	894 D		894 p	
	ν_3	PCl_2 s-stretch.	547 D		547 p	
	ν_4	PO ip-bend.	386 D		386 p	
	ν_5	PF bend.	330 D		330 p	
	ν_6	PCl_2 scis.	207 D		207 p	
a"	ν_7	PCl_2 a-stretch.	620 D		620 dp	
	ν_8	PO op-bend.	372 D		372 dp	
	ν_9	PCl_2 rock.	254 D		254 dp	

Reference

[1] R. M. L. Delwaulle and F. François, Comptes Rendus **222**, 550 (1946).

No. 303 Phosphoryl fluorodibromide $OPFBr_2$

Symmetry C_s **Symmetry number $\sigma = 1$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm $^{-1}$	*cm* $^{-1}$	*cm* $^{-1}$ (Liquid)	
a'	ν_1	PO stretch.	1303 D		1303 p	
	ν_2	PF stretch.	880 D		880 p	
	ν_3	PBr_2 s-stretch.	466 D		466 p	
	ν_4	PO ip-bend.	306 D		306 p	
	ν_5	PF bend.	273 D		273 p	
	ν_6	PBr_2 scis.	134 D		134 p	
a"	ν_7	PBr_2 a-stretch.	538 D		538 dp	
	ν_8	PO op-bend.	291 D		291 dp	
	ν_9	PBr_2 rock.	220 D		220 dp	

Reference

See No. 302 ($OPFCl_2$).

No. 304 Phosphorus pentafluoride PF_5

Symmetry D_{3h} Symmetry number $\sigma = 6$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Gas)	
a_1'	ν_1	PF_3 s–stretch.	816 B		816 (10) p	
	ν_2	PF_2 s–stretch.	648 C		648 (1b) p	
a_2''	ν_3	PF_2 a–stretch.	947 B	946.6 VS		
	ν_4	PF_3 op–deform.	575 B	575.1 M		
e'	ν_5	PF_3 d–stretch.	1024 B	1024 VS	1029 (1b)	
	ν_6	PF_3 d–deform.	533 B	532.5 M	535 (1sh) dp	
	ν_7	PF bend.	174 C		174 (1b) dp	
e''	ν_8	PF bend.	520 C		520 (1b) dp	

References

[1] IR. J. E. Griffiths, R. P. Carter, and R. R. Holmes, J. Chem. Phys. **41**, 863 (1964).
[2] IR. L. C. Hoskins, J. Chem. Phys. **42**, 2631 (1965).
[3] IR. J. E. Griffiths, J. Chem. Phys. **42**, 2632 (1965).
[4] IR.R. L. C. Hoskins and R. C. Lord, J. Chem. Phys. **46**, 2402 (1967).
[5] IR. R. M. Deiters and R. R. Holmes, J. Chem. Phys. **48**, 4796 (1968).
[6] R. I. W. Levin, J. Chem. Phys. **50**, 1031 (1969).
[7] Th. I. W. Levin, J. Mol. Spectry. **33**, 61 (1970).
[8] R. F. A. Miller and R. J. Capwell, Spectrochim. Acta **27A**, 125 (1971).

No. 305 Vanadium pentafluoride VF_5

Symmetry D_{3h} Symmetry number $\sigma = 6$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Gas)	
a_1'	ν_1	VF_3 s–stretch.	718 B		718 VS	
	ν_2	VF_2 s–stretch.	608 B		608 M	
a_2''	ν_3	VF_2 a–stretch.	784 B	784 S		
	ν_4	VF_3 op–deform.	331 B	331 W		
e'	ν_5	VF_3 d–stretch.	810 C	810 M	812 W	
	ν_6	VF_3 d–deform.	282 C	282 M	286 VW	
	ν_7	VF bend.	110 D	109.5 M	99 W	
e''	ν_8	VF bend.	336 B		336 M	

References

[1] IR. R. G. Cavell and H. C. Clark, Inorg. Chem. **3**, 1789 (1964).
[2] IR.R. H. H. Claassen and H. Selig, J. Chem. Phys. **44**, 4039 (1966).
[3] IR.R. I. R. Beattie, K. M. S. Livingston, G. A. Ozin, and D. J. Reynolds, J. Chem. Soc. A**1969**, 958.
[4] IR.R. H. Selig, J. H. Holloway, J. Tyson, and H. H. Claassen, J. Chem. Phys. **53**, 2559 (1970).

No. 306 Arsenic pentafluoride AsF_5

Symmetry D_{3h} **Symmetry number $\sigma = 6$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Gas)	
a_1'	ν_1	AsF_3 s-stretch.	734 C		734.3 VS, p	
	ν_2	AsF_2 s-stretch.	644 C		644 M, p?	
a_2''	ν_3	AsF_2 a-stretch.	787 B	787.4 VS		
	ν_4	AsF_3 op-deform.	400 B	400.4 S		
e'	ν_5	AsF_3 d-stretch.	811 B	811.4 VS	813 M, dp	
	ν_6	AsF_3 d-deform.	372 C	372 S	366	
					(Liquid)	
	ν_7	AsF bend.	123 C	123 W	130 M, dp	
e''	ν_8	AsF bend.	386 C		386 M, dp	

References

[1] IR.R. L. C. Hoskins and R. C. Lord, J. Chem. Phys. **46,** 2402 (1967).
[2] Th. I. W. Levin, J. Mol. Spectry. **33,** 61 (1970).
[3] R. H. Selig, J. H. Holloway, J. Tyson, and H. H. Claassen, J. Chem. Phys. **53,** 2559 (1970).
[4] IR. L. C. Hoskins and C. N. Perng, J. Chem. Phys. **55,** 5063 (1971).

No. 307 Iridium(VI) fluoride IrF_6

Symmetry O_h **Symmetry number $\sigma = 24$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Gas)	
a_{1g}	ν_1	Sym. stretch.	702 B	ia	701.7 VS, p	
e_g	ν_2	Deg. stretch.	645 C	ia	645 W, dp	
f_{1u}	ν_3	Deg. stretch.	720 B	719.8 S	ia	
	ν_4	Deg. deform.	276 B	276.0 S	ia	
f_{2g}	ν_5	Deg. deform.	267 C	ia	267 W, dp	
f_{2u}	ν_6	Deg. deform.	206 D	ia	ia	OC($\nu_2+\nu_6$, $\nu_2-\nu_6$, $\nu_5+\nu_6$). [1].

References

[1] IR.R. B. Weinstock and G. L. Goodman, Advan. Chem. Phys. **9,** 169 (1966), and references cited there.
[2] R. H. H. Claassen and H. Selig, Israel J. Chem. **7,** 449 (1969).
[3] IR. H. Kim, P. A. Souder, and H. H. Claassen, J. Mol. Spectry. **26,** 46 (1968).

No. 308 Sulfur chloride pentafluoride $SClF_5$
Symmetry C_{4v} Symmetry number $\sigma = 4$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1	ν_1	SF stretch.	855 B	854.6 VS	833 W, p	
	ν_2	SF_4 s–stretch.	707 B	707.2 VS	704 S, p	
	ν_3	SF_4 op–deform.	602 B	601.9 VS	603 W, p	
	ν_4	SCl stretch.	402 B	401.7 VS	403 VS, p	
b_1	ν_5	SF_4 a–stretch.	625 C	ia	625 M, dp	
	ν_6	SF_4 op–deform.	271 C	ia	271 M, dp	
b_2	ν_7	SF_4 ip–deform.	505 C	ia	505 W, dp	
e	ν_8	SF_4 d–stretch.	909 B	909.0 VS	927 W, dp	
	ν_9	SF bend.	579 B	579.0 M	584 VW, dp	
	ν_{10}	SF_4 ip–deform.	441 B	441.0 S	442 M, dp	
	ν_{11}	SCl bend.	397 B	396.5 S	396 S, dp	

References

[1] IR.R. L. H. Cross, H. L. Roberts, P. Goggin, and L. A. Woodward, Trans. Faraday Soc. **56**, 945 (1960).

[2] IR.R. J. E. Griffiths, Spectrochim. Acta **23A**, 2145 (1967).

No. 309 Tungsten chloride pentafluoride $WClF_5$
Symmetry C_{4v} Symmetry number $\sigma = 4$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1	ν_1	WF stretch.	743 C	743 M	744 VS, p	
	ν_2	WF_4 s–stretch.	703 C	703 VS	703 M, p	
	ν_3	WCl stretch.	400 C	400 VS	407 S, p	
	ν_4	WF_4 op–deform.	254 C	254 VS	257 W	
b_1	ν_5	WF_4 a–stretch.	644 D	ia	644 W	
	ν_6	WF_4 op–deform.	182 D	ia	182 W	
b_2	ν_7	WF_4 ip–deform.	377 D	ia	377 M, dp	
e	ν_8	WF_4 d–stretch.	671 C	671 S	661 M, dp	
	ν_9	WF bend.	302 C	302 M	307 M, dp	
	ν_{10}	WF_4 ip–deform.	278 C	278 S	290 W	
	ν_{11}	WCl bend.	228 C	228 S	227 W	

Reference

[1] IR.R. D. M. Adams, G. W. Fraser, D. M. Morris, and R. D. Peacock, J. Chem. Soc. A 1131 (1968).

No. 310 Cyanogen fluoride FCN

Symmetry $C_{\infty v}$ **Symmetry number $\sigma = 1$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1}	
σ^+	ν_1	CF stretch.	1077 A	1076.52		
π	ν_2	Deform.	451 A	451.32		
σ^+	ν_3	CN stretch.	2323 C	2323		

References

[1] IR. R. E. Dodd and R. Little, Spectrochim. Acta **16,** 1083 (1960).
[2] IR. A. R. H. Cole, L. Isaacson, and R. C. Lord, Spectrochim. Acta **23,** 86 (1967).
[3] Th. A. Ruoff, Spectrochim. Acta **26A,** 545 (1970).

No. 311 Cyanogen iodide ICN

Symmetry $C_{\infty v}$ **Symmetry number $\sigma = 1$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1}	
σ^+	ν_1	CI stretch.	486 C	485.8		
π	ν_2	Deform.	305 C	304.5		
σ^+	ν_3	CN stretch.	2188 C	2188.0		

References

[1] IR. S. Hemple and E. R. Nixon, J. Chem. Phys. **47,** 4273 (1967).
[2] Th. A. Ruoff, Spectrochim. Acta **26A,** 545 (1970).

No. 312 Carbonyl fluoride COF_2

Symmetry C_{2v} **Symmetry number $\sigma = 2$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1	ν_1	CO stretch.	1928 C	1928 VS	1944 VW	
	ν_2	CF_2 s-stretch.	965 B	965 VS	965 VS	
	ν_3	CF_2 deform.	584 C	584 M	571 W	
b_1	ν_4	CF_2 a-stretch.	1249 B	1249 VS	1238 VW	
	ν_5	CO deform.	626 C	626 M	620 M	
b_2	ν_6	Op-deform.	774 B	774 M	771 VW	

References

[1] IR.R. A. H. Nielsen, T. G. Burke, P. J. H. Woltz, and E. A. Jones, J. Chem. Phys. **20,** 596 (1952).
[2] Th. J. Overend and J. R. Scherer, J. Chem. Phys. **32,** 1296 (1960).

No. 313 Carbonyl chloride $COCl_2$

Symmetry C_{2v} Symmetry number $\sigma = 2$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm $^{-1}$	cm $^{-1}$ (Gas)	cm $^{-1}$ (Liquid)	
a_1	ν_1	CO stretch.	1827 B	1827 VS	1807 M	
	ν_2	CCl_2 s-stretch.	567 C	567 M	573 VS	
	ν_3	CCl_2 deform.	285 C	285 W	302 S	
b_1	ν_4	CCl_2 a-stretch.	849 B	849 S	832 VW	
	ν_5	CO deform.	440 C	440 M	442 M	
b_2	ν_6	Op-deform.	580 C	580 M		

References

[1] IR.R.	A. H. Nielsen, T. G. Burke, P. J. H. Woltz, and E. A. Jones, J. Chem. Phys. **20**, 596 (1952).
[2] IR.	E. Catalano and K. S. Pitzer, J. Amer. Chem. Soc. **80**, 1054 (1958).
[3] IR.R.	J. Overend and J. C. Evans, Trans. Faraday Soc. **55**, 1817 (1959).
[4] Th.	J. Overend and J. R. Scherer, J. Chem. Phys. **32**, 1296 (1960).

No. 314 Carbonyl bromide $COBr_2$

Symmetry C_{2v} Symmetry number $\sigma = 2$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm $^{-1}$	cm $^{-1}$ (Gas)	cm $^{-1}$ (Liquid)	
a_1	ν_1	CO stretch.	1828 B	1828 VS		
	ν_2	CBr_2 s-stretch.	425 C	425 M	429 S	
	ν_3	CBr_2 deform.	181 D		181 S	
b_1	ν_4	CBr_2 a-stretch.	757 C	787 VS 747 VS		FR($\nu_2+\nu_5$).
	ν_5	CO deform.	350 C	350 VW	350 M, b	
b_2	ν_6	Op-deform.	512 B	512 M		

References

[1] IR.R.	J. Overend and J. C. Evans, Trans. Faraday Soc. **15**, 1817 (1959).
[2] Th.	J. Overend and J. R. Scherer, J. Chem. Phys. **32**, 1296 (1960).

No. 315 Thiocarbonyl fluoride SCF_2

Symmetry C_{2v} **Symmetry number $\sigma = 2$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	CS stretch.	1368 C	1368 VS		
	ν_2	CF_2 s-stretch.	787 C	787 M		
	ν_3	CF_2 scis.	526 C	526 M		
b_1	ν_4	CF_2 a-stretch.	1189 C	1189 S		
	ν_5	CF_2 rock.	417 C	417 VW		
b_2	ν_6	CF_2 wag.	622 C	622 W		

Reference

[1] IR. A. J. Downs, Spectrochim. Acta **19**, 1165 (1963).

No. 316 Isocyanic acid HNCO

Symmetry C_s **Symmetry number $\sigma = 1$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Liquid)	
a'	ν_1	NH stretch.	3531 C	3531 S	3410	
	ν_2	CO stretch.	2274 C	2274 VS		
	ν_3	CN stretch.	1327 C	1327 W	1318	
	ν_4	NH bend.	762 B[a]	777.1 S		
	ν_5	NCO deform.	643 B[a]	659.8 M		
a''	ν_6	NCO deform.	610 B[a]	577.5 M		

[a] Three fundamentals, ν_4, ν_5, and ν_6, are strongly coupled through Coriolis interaction. The unperturbed frequencies are given in this column [3].

References

[1] R. G. Herzberg and C. Reid, Disc. Faraday Soc. **9**, 92 (1950).
[2] IR. C. Reid, J. Chem. Phys. **18**, 1544 (1954).
[3] IR. R. A. Ashby and R. L. Werner, J. Mol. Spectry. **18**, 184 (1965).

No. 317 Isocyanic acid–d DNCO

Symmetry C_s **Symmetry number $\sigma = 1$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	*cm*$^{-1}$ (Gas)	*cm*$^{-1}$	
a'	ν_1	ND stretch.	2635 B	2634.9		
	ν_2	CO stretch.	2235 C	2235		
	ν_3	CN stretch.	1310 C	1310		
	ν_4	ND bend.	758 C[a]	766.8		
	ν_5	CNO deform.	458 C[a]	460		
a''	ν_6	CNO deform.	603 B[a]	602.9		

[a] See footnote of HNCO.

Reference

[1] IR. R. A. Ashby and R. L. Werner, Spectrochim. Acta **22**, 1345 (1966).

No. 318 Carbonyl chlorofluoride COClF

Symmetry C_s **Symmetry number $\sigma = 1$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	*cm*$^{-1}$ (Gas)	*cm*$^{-1}$ (Liquid)	
a'	ν_1	CO stretch.	1868 C	1876 VS 1847 VS	1858 M 1832 M	FR($\nu_2+\nu_3$).
	ν_2	CF stretch.	1095 B	1095 S	1085 VW	
	ν_3	CCl stretch.	776 C	776 M	765 VS	
	ν_4	CO deform.	501 C	501 W	506 S	
	ν_5	CClF deform.	415 C	415 VW	410 M	
a''	ν_6	Op–deform.	667 B	667 M	665 VW	

References

See No. 312 (COF_2).

No. 319 Carbonyl bromochloride COBrCl

Symmetry C_s **Symmetry number $\sigma = 1$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Liquid)	
a'	ν_1	CO stretch.	1828 B	1828 VS		
	ν_2	CCl stretch.	806 C	806 VS		
	ν_3	CBr stretch.	517 C	517 M	518 M	
	ν_4	CO deform.	374 C	374 W	372 M	
	ν_5	CBrCl deform.	240 D		240 S	
a''	ν_6	Op–deform.	547 B	547 W		

References

[1] IR.R. J. Overend and J. C. Evans, Trans. Faraday Soc. **55,** 1817 (1959).
[2] Th. J. Overend and J. R. Scherer, J. Chem. Phys. **32,** 1296 (1960).

No. 320 Trifluoromethane–d CDF_3

Symmetry C_{3v} **Symmetry number $\sigma = 3$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	CD stretch.	2261 B	2261.0 S		
	ν_2	CF_3 s–stretch.	1111 B	1110.6 M		
	ν_3	CF_3 s–deform.	694 B	694.2 M		
e	ν_4	CD bend.	1202 D	1202.2 M		FR($\nu_3+\nu_6$).
	ν_5	CF_3 d–stretch.	975 B	975.1 S		
	ν_6	CF_3 d–deform.	502 B	502.4 M		

References

[1] IR. S. R. Polo and M. K. Wilson, J. Chem. Phys. **21,** 1129 (1953).
[2] IR. C. C. Costain, J. Mol. Spectry. **9,** 317 (1962).
[3] IR.Th. A. Ruoff, H. Bürger, and S. Biedermann, Spectrochim. Acta **27A,** 1359, 1377 (1971).

No. 321 Borine Carbonyl $^{10}BH_3CO$

Symmetry C_{3v} **Symmetry number $\sigma = 3$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm $^{-1}$	*cm* $^{-1}$ (Gas)	*cm* $^{-1}$	
a_1	ν_1	BH_3 s-stretch.	2387 D	2387 M		
				(solid)		
	ν_2	CO stretch.	2166 D	2166.0 VS		
	ν_3	BH_3 s-deform.	1083 C	1083.1 S		
	ν_4	BC stretch.	707 B	707.0 S		
e	ν_5	BH_3 d-stretch.	2456 D	2456 VS		
	ν_6	BH_3 d-deform.	1115 E	1114.8 S		
	ν_7	BH_3 rock.	819 B	818.8 M		
	ν_8	BCO bend.	314 B	313.7 S		

References

[1] IR. R. D. Cowan, J. Chem. Phys. **18,** 1101 (1950).

[2] IR.Th. G. W. Bethke and M. K. Wilson, J. Chem. Phys. **26,** 1118 (1957).

No. 322 Borine Carbonyl-d_3 $^{10}BD_3CO$

Symmetry C_{3v} **Symmetry number $\sigma = 3$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm $^{-1}$	*cm* $^{-1}$ (Gas)	*cm* $^{-1}$	
a_1	ν_1	BD_3 s-stretch.	1695 C	1694.8 M		
	ν_2	CO stretch.	2169 D	2169.0 VS		
	ν_3	BD_3 s-deform.	888 D	888.4 W		
				(solid)		
	ν_4	BC stretch.	630 B	629.5 S		
e	ν_5	BD_3 d-stretch.	1852 C	1852 S		
	ν_6	BD_3 d-deform.	802 B	801.5 W		
	ν_7	BD_3 rock.	718 B	718.0 S		
	ν_8	BCO bend.	266 B	266.0 S		

References

See No. 321 ($^{10}BH_3CO$).

No. 323 Borine Carbonyl $^{11}BH_3CO$

Symmetry C_{3v} **Symmetry number $\sigma = 3$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm $^{-1}$	*cm* $^{-1}$ (Gas)	*cm* $^{-1}$ (Liquid)	
a_1	ν_1	BH$_3$ s–stretch.	2380 C	2379 M	2380 S, p	
				(solid)		
	ν_2	CO stretch.	2165 D	2164.7 VS	2169 S, p	
	ν_3	BH$_3$ s–deform.	1073 C	1073.4 S	1073 S, p	
	ν_4	BC stretch.	691 B	691.4 S	692 W, p	
e	ν_5	BH$_3$ d–stretch.	2444 D	2444 VS	2434 S	
	ν_6	BH$_3$ d–deform.	1106 E	1105.8 S	1101 M	
	ν_7	BH$_3$ rock.	809 B	809.3 M	816 W	
	ν_8	BCO bend.	313 B	313.2 S	317 M	

References

[1] IR. R. D. Cowan, J. Chem. Phys. **18,** 1101 (1950).
[2] IR.Th. G. W. Bethke and M. K. Wilson, J. Chem. Phys. **26,** 1118 (1957).
[3] R.Th. R. C. Taylor, J. Chem. Phys. **26,** 1131 (1957).

No. 324 Borine Carbonyl–d$_3$ $^{11}BD_3CO$

Symmetry C_{3v} **Symmetry number $\sigma = 3$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm $^{-1}$	*cm* $^{-1}$ (Gas)	*cm* $^{-1}$ (Liquid)	
a_1	ν_1	BD$_3$ s–stretch.	1679 C	1679.0 M	1678 S	
	ν_2	CO stretch.	2169 D	2168.5 VS	2169 S	
	ν_3	BD$_3$ s–deform.	860 C	867.7 W	860 M	
				(solid)		
	ν_4	BC stretch.	625 B	624.8 S	619 M	
e	ν_5	BD$_3$ d–stretch.	1840 C	1840 S	1825 S	
	ν_6	BD$_3$ d–deform.	801 B	801.3 W	808 M	
	ν_7	BD$_3$ rock.	709 B	709.3 S	706 W	
	ν_8	BCO bend.	266 B	266.0 S	264 W	

References

See No. 323 ($^{11}BH_3CO$).

No. 325 Dichloroacetylene C_2Cl_2
Symmetry $D_{\infty h}$ **Symmetry number $\sigma = 2$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm $^{-1}$	cm $^{-1}$ (Gas)	cm $^{-1}$ (Liquid)	
σ_g^+	ν_1	CC stretch.	2234 D	ia	2234 S, p	
	ν_2	CCl stretch.	477 D	ia	477 M, p	
σ_u^+	ν_3	CCl stretch.	988 C	988 VS	ia	
π_g	ν_4	CCCl deform.	333 D	ia	333 VS, dp	
π_u	ν_5	CCCl deform.	172 C	172 S	ia	

Reference
[1] IR.R. P. Klaboe and E. Kloster–Jensen, Spectrochim. Acta **26A**, 1567 (1970).

No. 326 Dibromoacetylene C_2Br_2
Symmetry $D_{\infty h}$ **Symmetry number $\sigma = 2$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm $^{-1}$	cm $^{-1}$ (Gas)	cm $^{-1}$ (C_6H_6 soln.)	
σ_g^+	ν_1	CC stretch.	2185 D	ia	2185 VS, p	
	ν_2	CBr stretch.	267 D	ia	267 M, p	
σ_u^+	ν_3	CBr stretch.	832 C	832 VS	ia	
π_g	ν_4	CCBr deform.	311 D	ia	311 VS, dp	
π_u	ν_5	CCBr deform.	137 C	137 S	ia	

Reference
See No. 325 (C_2Cl_2).

No. 327 Diiodoacetylene C_2I_2

Symmetry $D_{\infty h}$ **Symmetry number $\sigma = 2$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1}	cm^{-1} (C_6H_6 soln.)	
σ_g^+	ν_1	CC stretch.	2118 D	ia	2118 VS, p	
	ν_2	CI stretch.	190 D	ia	190 S, p	
σ_u^+	ν_3	CI stretch.	720 D	720 VS (CS_2 soln.)	ia	
π_g	ν_4	CCI deform.	296 D	ia	296 VS, dp	
π_u	ν_5	CCI deform.	132 D	132 M (C_6H_6 soln.)	ia	

References

[1] IR.R. A. G. Meister and F. F. Cleveland, J. Chem. Phys. **17,** 212 (1949).

[2] IR.R. P. Klaboe and E. Kloster–Jensen, Spectrochim. Acta **26A,** 1567 (1970).

No. 328 Bromochloroacetylene C_2ClBr

Symmetry $C_{\infty v}$ **Symmetry number $\sigma = 1$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (C_6H_6 soln.)	
σ^+	ν_1	CC stretch.	2223 C	2223 VS	2205 M, p	
	ν_2	CCl stretch.	923 C	923 VS	917 VS	
	ν_3	CBr stretch.	389 C	389 VW	388 S, p (CCl_4 soln.)	
π	ν_4	CCCl deform.	326 D		326 VS, dp (CCl_4 soln.)	
	ν_5	CCBr deform.	152 C	152 S	165 M	

Reference

[1] IR.R. P. Klaboe and E. Kloster–Jensen, Spectrochim. Acta **26A,** 1567 (1970).

No. 329 Chloroiodoacetylene C_2ClI

Symmetry $C_{\infty v}$ **Symmetry number $\sigma = 1$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (C_6H_6 soln.)	
σ^+	ν_1	CC stretch.	2191 C	2191 VS	2178 VS, p	
	ν_2	CCl stretch.	886 C	886 VS	880 VW	
	ν_3	CI stretch.	276 D		276 M, p	
π	ν_4	CCCl deform.	325 D		325 VS, dp	
	ν_5	CCI deform.	135 C	135 S	145 VW (CCl_4 soln.)	

Reference

See No. 328 (C_2ClBr).

No. 330 trans-1,2-Difluoroethylene CHFCHF

Symmetry C_{2h} **Symmetry number $\sigma = 2$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_g	ν_1	CH stretch.	3111 C	ia	3111 VS, p	
	ν_2	CC stretch.	1694 C	ia	1694 VS, p	
	ν_3	CH bend.	1286 C	ia	1286 S, p	
	ν_4	CF stretch.	1123 C	ia	1123 M, p	
	ν_5	CCF deform.	548 C	ia	548 S, p	
a_u	ν_6	CH bend.	875 B	875 S	ia	
	ν_7	Torsion	329 D	333 M (Xe Matrix) 325 M (Xe Matrix)	ia	
b_g	ν_8	CH bend.	788 C	ia	788 S, dp	
b_u	ν_9	CH stretch.	3114 C	3114 M	ia	
	ν_{10}	CH bend.	1274 C	1274 M	ia	
	ν_{11}	CF stretch.	1159 C	1159 VS	ia	
	ν_{12}	CCF deform.	341 D	341 M (Xe Matrix)	ia	

Reference

[1] IR.R. N. C. Craig and J. Overend, J. Chem. Phys. **51**, 1127 (1969).

No. 331 trans-1,2-Difluoroethylene-d_1 CHFCDF

Symmetry C_s **Symmetry number $\sigma = 1$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm $^{-1}$	cm $^{-1}$ (Gas)	cm $^{-1}$ (Liquid)	
a'	ν_1	CH stretch.	3110 C	3110 M	3112 S, p	
	ν_2	CD stretch.	2335 C	2335 M	2333 M, p	
	ν_3	CC stretch.	1674 C		1674 S, p	
	ν_4	CH bend.	1274 C	1274 M	1274 M, p	
	ν_5	CF stretch.	1166 C	1166 VS	1155 VW	
	ν_6	CF stretch.	1138 C	1138 M	1119 M, p	
	ν_7	CD bend.	940 C	940 M	941 M, dp	
	ν_8	CCF deform.	542 C		542 S, p	
	ν_9	CCF deform.	332 D	332 M		
a''	ν_{10}	CH bend.	828 B	828 S	829 M, dp	
	ν_{11}	CD bend.	673 B	673 M	673 M, dp	
	ν_{12}	Torsion	316 C	316 S		

Reference

See No. 330 (CHFCHF).

No. 332 trans-1,2-Difluoroethylene-d_2 CDFCDF

Symmetry C_{2h} **Symmetry number $\sigma = 2$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm $^{-1}$	cm $^{-1}$ (Gas)	cm $^{-1}$ (Liquid)	
a_g	ν_1	CD stretch.	2355 C	ia	2355 S, p	
	ν_2	CC stretch.	1642 C	ia	1642 VS, p	
	ν_3	CF stretch.	1109 C	ia	1109 S, p	
	ν_4	CD bend.	935 C	ia	935 M, dp	
	ν_5	CCF deform.	538 C	ia	538 S, p	
a_u	ν_6	CD bend.	651 B	651 S	ia	
	ν_7	Torsion	309 C	309 S	ia	
b_g	ν_8	CD bend.	685 C	ia	685 S, dp	
b_u	ν_9	CD stretch.	2312 C	2312 M	ia	
	ν_{10}	CF stretch.	1173 C	1173 VS	ia	
	ν_{11}	CD bend.	942 C	942 M	ia	
	ν_{12}	CCF deform.	324 D	324 M	ia	

References

[1] R. N. C. Craig and J. Overend, Spectrochim. Acta **20,** 1561 (1964).
[2] IR.R. N. C. Craig and J. Overend, J. Chem. Phys. **51,** 1127 (1969).

No. 333 1,4–Dioxane $C_4H_8O_2$
Symmetry C_{2h} **Symmetry number $\sigma = 2$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1}	cm^{-1}	
				(Liquid)	(Liquid)	
a_g	ν_1	CH_2 a–stretch.	2966 C	ia	2966 (10)p	
	ν_2	CH_2 s–stretch.	2855 C	ia	2855 (8)p	
	ν_3	CH_2 scis.	1443 C	ia	1443 (8)p	
	ν_4	CH_2 wag.	1334 C	ia	1334 (2)p	
	ν_5	CH_2 twist.	1303 C	ia	1303 (8)p	
	ν_6	CH_2 rock.	1127 C	ia	1127 (3)p	
	ν_7	CC stretch.	1015 C	ia	1015 (6)p	
	ν_8	CO stretch.	834 C	ia	834 (8)p	
	ν_9	OCC deform.	503 E	ia		CF[2].
	ν_{10}	COC deform.	427 C	ia	433 (2)p 422 (1)	FR($2\nu_{27}$).
a_u	ν_{11}	CH_2 a–stretch.	2974 C	2974 M	ia	
	ν_{12}	CH_2 s–stretch.	2867 C	2867 S	ia	
	ν_{13}	CH_2 scis.	1457 C	1457 M	ia	
	ν_{14}	CH_2 wag.	1367 C	1367 W	ia	
	ν_{15}	CH_2 twist.	1264 C	1264 S	ia	
	ν_{16}	CO stretch.	1123 C	1123 VS	ia	
	ν_{17}	CH_2 rock.	1088 C	1088 M	ia	
	ν_{18}	CC stretch.	894 C	894 M	ia	
	ν_{19}	OCC deform.	224 C	224 VW	ia	
b_g	ν_{20}	CH_2 a–stretch.	2966 C	ia	2966 (10)p	SF(ν_1).
	ν_{21}	CH_2 s–stretch.	2855 C	ia	2855 (8)p	SF(ν_2).
	ν_{22}	CH_2 scis.	1461 C	ia	1461 (2)dp	
	ν_{23}	CH_2 wag.	1396 C	ia	1396 (1)	
	ν_{24}	CH_2 twist.	1216 C	ia	1216 (5)dp	
	ν_{25}	CO stretch.	1109 C	ia	1109 (3)dp	
	ν_{26}	CH_2 rock.	852 C	ia	852 (1)dp	
	ν_{27}	OCC deform.	486 C	ia	486 (4)dp	
b_u	ν_{28}	CH_2 a–stretch.	2974 C	2974 M	ia	SF(ν_{19}).
	ν_{29}	CH_2 s–stretch.	2867 C	2867 S	ia	SF(ν_{20}).
	ν_{30}	CH_2 scis.	1457 C	1457 M	ia	
	ν_{31}	CH_2 wag.	1377 C	1377 W	ia	
	ν_{32}	CH_2 twist.	1296 C	1296 M	ia	
	ν_{33}	CH_2 rock.	1052 C	1052 W	ia	
	ν_{34}	CO stretch.	871 C	871 S	ia	
	ν_{35}	OCC deform.	610 C	610 M	ia	
	ν_{36}	COC deform.	276 C	276 M	ia	

References

[1] IR.R. F. E. Malherbe and H. J. Bernstein, J. Amer. Chem. Soc. **74**, 4408 (1952), and references cited there.
[2] IR.Th. R. G. Snyder and G. Zerbi, Spectrochim. Acta **23A**, 391 (1967).

No. 334 Hexacarbonylchromium(0) $Cr(^{12}C^{16}O)_6$

Symmetry O_h **Symmetry number $\sigma = 24$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (CCl_4 soln.)	
a_{1g}	ν_1	CO stretch.	2112 C	ia	2112.4 M	
	ν_2	CrC stretch.	381 C	ia	381.2 S	
e_g	ν_3	CO stretch.	2018 C	ia	2018.4 M	
	ν_4	CrC stretch.	394 D	ia	394 W	
f_{1g}	ν_5	CrCO bend.	364 D	ia	ia	OC($\nu_5+\nu_7$).
f_{1u}	ν_6	CO stretch.	2000 B	2000.4 VS	ia	
	ν_7	CrC stretch.	668 B	668.1 VS	ia	
	ν_8	CrCO bend.	441 B	440.5 S	ia	
	ν_9	CCrC deform.	98 B	97.8 M	ia	
f_{2g}	ν_{10}	CrCO bend.	533 D	ia	533.1 W (solid)	
	ν_{11}	CCrC deform.	114 D	ia	114.2 S (solid)	
f_{2u}	ν_{12}	CrCO bend.	511 D	ia	ia	OC($\nu_{10}+\nu_{12}$, $\nu_5+\nu_{12}$).
	ν_{13}	CCrC deform.	68 E	ia	ia	OC($\nu_3+\nu_{13}$).

References

[1] IR. N. J. Hawkins, H. C. Mattraw, W. W. Sabol, and D. R. Carpenter, J. Chem. Phys. **23**, 2422 (1955).
[2] Th. H. Murata and K. Kawai, J. Chem. Phys. **27**, 605 (1957).
[3] IR.Th. L. H. Jones, Spectrochim. Acta **19**, 329 (1963).
[4] IR.Th. J. M. Smith and L. H. Jones, J. Mol. Spectry. **20**, 248 (1966).
[5]IR.R.Th. L. H. Jones, R. S. McDowell, and M. Goldblatt, Inorg. Chem. **8**, 2349 (1969).

No. 335 Hexacarbonylmolybdenum (0) $Mo(^{12}C^{16}O)_6$

Symmetry O_h Symmetry number $\sigma = 24$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (CCl_4 soln.)	
a_{1g}	ν_1	CO stretch.	2117 C	ia	2116.7 M	
	ν_2	MoC stretch.	402 C	ia	402.2 S	
e_g	ν_3	CO stretch.	2019 C	ia	2018.8 M	
	ν_4	MoC stretch.	392 C	ia	392 W	
f_{1g}	ν_5	MoCO bend.	342 D	ia	ia	OC($\nu_5+\nu_7$).
f_{1u}	ν_6	CO stretch.	2003 B	2003.0 VS	ia	
	ν_7	MoC stretch.	596 B	595.6 VS	ia	
	ν_8	MoCO bend.	367 B	367.2 S	ia	
	ν_9	CMoC deform.	82 B	81.6 M	ia	
f_{2g}	ν_{10}	MoCO bend.	477 D	ia	476.5 W (solid)	
	ν_{11}	CMoC deform.	104 D	ia	103.7 S (solid)	
f_{2u}	ν_{12}	MoCO bend.	507 D	ia	ia	OC($\nu_5+\nu_{12}$, $\nu_{10}+\nu_{12}$).
	ν_{13}	CMoC deform.	60 E	ia	ia	OC($\nu_3+\nu_{13}$, $\nu_{10}+\nu_{13}$).

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[6]IR.R.Th. L. H. Jones, R. S. McDowell, and M. Goldblatt, Inorg. Chem. **8**, 2349 (1969).

No. 336 Hexacarbonyltungsten(0) $W(^{12}C^{16}O)_6$

Symmetry O_h **Symmetry number $\sigma = 24$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm⁻¹	cm⁻¹ (Gas)	cm⁻¹ (CS$_2$ soln.)	
a_{1g}	ν_1	CO stretch.	2117 C	ia	2116.6 M	
	ν_2	WC stretch.	427 C	ia	427.1 S	
e_g	ν_3	CO stretch.	2010 C	ia	2009.8 M	
	ν_4	WC stretch.	412 C	ia	412 W	
f_{1g}	ν_5	WCO bend.	362 D	ia	ia	OC($\nu_5+\nu_7$).
f_{1u}	ν_6	CO stretch.	1998 B	1997.6 VS	ia	
	ν_7	WC stretch.	587 B	586.6 VS	ia	
	ν_8	WCO bend.	374 B	374.4 S	ia	
	ν_9	CWC deform.	82 C	82.0 M	ia	
f_{2g}	ν_{10}	WCO bend.	485 D	ia	485.0 W (solid)	
	ν_{11}	CWC deform.	108 D	ia	107.6 S (solid)	
f_{2u}	ν_{12}	WCO bend.	521 D	ia	ia	OC($\nu_5+\nu_7$, $\nu_{10}+\nu_{12}$).
	ν_{13}	CWC deform.	61 E	ia	ia	OC($\nu_3+\nu_{13}$).

References

[1] IR.Th. L. H. Jones, Spectrochim. Acta **19**, 329 (1963).
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APPENDIX I

A. Structure–Symmetry Index

This index and the one which follows cover the entire list of compounds analyzed so far under this project, and presented in the Tables of Molecular Vibrational Frequencies, Consolidated Volume [2], Part 5[3] and the present publication.

Here the 336 molecules are ordered by structural and symmetry factors, following the principles set forth in ref [2]. Name, chemical formula and Table Number are listed. Tables numbered 1 through 223 may be found in ref [2], tables numbered 224 through 281 in ref [3], and tables numbered 282 through 336 in the present increment.

C_0–triatomic molecules

Nitrous oxide	$^{14}N_2O$	1
Nitrous oxide	$^{14}N^{15}NO$	2
Nitrous oxide	$^{15}N_2O$	3
Nitrogen dioxide	$^{14}NO_2$	224
Nitrogen dioxide	$^{15}NO_2$	225
Water	H_2O	4
Water	$H_2{}^{18}O$	282
Water–d_1	HDO	5
Water–d_2	D_2O	6
Oxygen difluoride	F_2O	7
Oxygen dichloride	Cl_2O	8
Hydrogen sulfide	H_2S	9
Deuterium sulfide	D_2S	10
Sulfur dioxide	$^{32}S^{16}O_2$	11
Sulfur dioxide	$S^{18}O_2$	283
Sulfur dichloride	SCl_2	226
Hydrogen selenide	H_2Se	12
Hydrogen deuterium selenide	HDSe	13
Nitrosyl fluoride	$^{16}O^{14}NF$	227
Nitrosyl fluoride	$^{16}O^{15}NF$	228
Nitrosyl fluoride	$^{18}O^{14}NF$	229
Nitrosyl fluoride	$^{18}O^{15}NF$	230
Nitrosyl chloride	$^{16}O^{14}NCl$	231
Nitrosyl chloride	$^{16}O^{15}NCl$	232
Nitrosyl chloride	$^{18}O^{14}NCl$	233
Nitrosyl chloride	$^{18}O^{15}NCl$	234
Nitrosyl bromide	$^{16}O^{14}NBr$	235
Nitrosyl bromide	$^{16}O^{15}NBr$	236
Nitrosyl bromide	$^{18}O^{15}NBr$	237
Hypochlorous acid	HOCl	284
Hypochlorous acid–d	DOCl	285
Thionitrosyl–S–fluoride	NSF	286
Thionitrosyl–S–chloride	NSCl	287

C_0–four–atomic molecules

Boron trifluoride	$^{10}BF_3$	238
Boron trifluoride	$^{11}BF_3$	239
Sulfur trioxide	SO_3	240
Ammonia	NH_3	14
Ammonia–d_3	ND_3	15
Ammonia–t_3	NT_3	291
Nitrogen trifluoride	NF_3	16
Phosphine	PH_3	17
Phosphine–d_3	PD_3	18
Phosphorus trifluoride	PF_3	19
Phosphorus trichloride	PCl_3	20
Arsine	AsH_3	21
Arsine–d_3	AsD_3	22
Arsenic trifluoride	AsF_3	292
Stibine	SbH_3	23
Stibine–d_3	SbD_3	24
Trans–1,2–Difluorodiazine	N_2F_2	288
Nitryl fluoride	$F^{14}NO_2$	241
Nitryl fluoride	$F^{15}NO_2$	242
Nitryl chloride	$Cl^{14}NO_2$	243
Nitryl chloride	$Cl^{15}NO_2$	244
Chlorine trifluoride	ClF_3	289
Bromine trifluoride	BrF_3	290
Hydrogen peroxide	H_2O_2	247
Hydrogen persulfide	H_2S_2	293
Difluoro disulfane	F_2S_2	294
Hydrazoic acid	HN_3	245
Hydrazoic acid–d_1	DN_3	246
Difluoroamine	NF_2H	295

C_0–five–atomic molecules

Thionyl fluoride	SOF_2	248
Thionyl chloride	$SOCl_2$	249
Thionyl bromide	$SOBr_2$	250
Silane	SiH_4	25
Silane–d_2	SiH_2D_2	26
Silane–d_3	$SiHD_3$	27
Silane–d_4	SiD_4	28
Silicon tetrafluoride	SiF_4	29
Silicon tetrachloride	$SiCl_4$	30
Silicon tetrabromide	$SiBr_4$	31
Silicon tetraiodide	SiI_4	32
Germane	GeH_4	33
Germane–d_1	GeH_3D	34
Germane–d_2	GeH_2D_2	35
Germane–d_3	$GeHD_3$	36
Germane–d_4	GeD_4	37
Germanium tetrachloride	$GeCl_4$	38
Germanium tetrabromide	$GeBr_4$	39
Tin (IV) chloride	$SnCl_4$	40
Tin (IV) bromide	$SnBr_4$	41
Ruthenium tetroxide	RuO_4	296
Osmium tetroxide	$Os^{16}O_4$	297
Osmium tetroxide	$Os^{18}O_4$	298
Silyl fluoride	SiH_3F	42
Silyl chloride	SiH_3Cl	43
Silyl bromide	SiH_3Br	44
Trifluorosilane	$SiHF_3$	251
Trifluorosilane–d	$SiDF_3$	252
Trichlorosilane	$SiHCl_3$	253

Trichlorosilane–d	$SiDCl_3$	254
Tribromosilane	$SiHBr_3$	255
Bromotrichlorosilane	$SiBrCl_3$	45
Trichloroiodosilane	$SiCl_3I$	46
Tribromochlorosilane	$SiBr_3Cl$	47
Chlorotriiodosilane	$SiClI_3$	48
Phosphoryl fluoride	POF_3	256
Phosphoryl chloride	$POCl_3$	257
Phosphoryl bromide	$POBr_3$	258
Germyl fluoride	GeH_3F	259
Germyl fluoride–d_3	GeD_3F	260
Germyl chloride	GeH_3Cl	261
Germyl chloride–d_3	GeD_3Cl	262
Germyl bromide	GeH_3Br	263
Germyl bromide–d_3	GeD_3Br	264
Germyl iodide	GeH_3I	265
Germyl iodide–d_3	GeD_3I	266
Trichlorogermane	$GeHCl_3$	267
Tribromogermane	$GeHBr_3$	268
Sulfuryl fluoride	SO_2F_2	269
Sulfuryl chloride	SO_2Cl_2	270
Dichlorosilane	SiH_2Cl_2	299
Dichlorosilane–d_2	SiD_2Cl_2	300
Dibromosilane	SiH_2Br_2	301
Dibromodichlorosilane	$SiBr_2Cl_2$	49
Selenium dioxide difluoride	SeO_2F_2	271
Phosphoryl fluorodichloride	$OPFCl_2$	302
Phosphoryl fluorodibromide	$OPFBr_2$	303

C_0–six–atomic molecules

Phosphorus pentafluoride	PF_5	304
Vanadium pentafluoride	VF_5	305
Arsenic pentafluoride	AsF_5	306

C_0–seven–atomic molecules

Sulfur hexafluoride	SF_6	50
Selenium hexafluoride	SeF_6	51
Molybdenum (VI) fluoride	MoF_6	52
Tellurium hexafluoride	TeF_6	272
Tungsten (VI) fluoride	WF_6	53
Iridium fluoride	IrF_6	307
Uranium (VI) fluoride	VF_6	54
Sulfur chloride pentafluoride	$SClF_5$	308
Tungsten chloride pentafluoride	$WClF_5$	309

C_0–eight–atomic molecules

Digermane	GeH_3GeH_3	273
Digermane–d_6	GeD_3GeD_3	274
Diborane	$^{10}B_2H_6$	55
Diborane	$^{11}B_2H_6$	56
Diborane	$^{10}B_2D_6$	57

C_1–triatomic molecules

Carbon dioxide	$^{12}CO_2$	58
Carbon dioxide	$^{13}CO_2$	59
Carbon disulfide	CS_2	60
Hydrogen cyanide	HCN	62
Deuterium cyanide	DCN	63
Cyanogen fluoride	FCN	310
Cyanogen chloride	$^{35}ClCN$	64
Cyanogen chloride	$^{37}ClCN$	65
Cyanogen bromide	$^{79}BrCN$	66
Cyanogen bromide	$^{81}BrCN$	67
Cyanogen iodide	ICN	311
Carbonyl sulfide	COS	61

C_1–four–atomic molecules

Formaldehyde	H_2CO	68
Formaldehyde–d_1	HDCO	69
Formaldehyde–d_2	D_2CO	70
Carbonyl fluoride	COF_2	312
Carbonyl chloride	$COCl_2$	313
Carbonyl bromide	$COBr_2$	314
Thiocarbonyl fluoride	SCF_2	315
Isocyanic acid	HNCO	316
Isocyanic acid–d	DNCO	317
Carbonyl chlorofluoride	COClF	318
Carbonyl bromochloride	COBrCl	319

C_1–five–atomic molecules

Methane	CH_4	71
Methane–d_1	CH_3D	72
Methane–d_2	CH_2D_2	73
Methane–d_3	CHD_3	74
Methane–d_4	CD_4	75
Carbon tetrafluoride	CF_4	76
Carbon tetrachloride	CCl_4	77
Carbon tetrabromide	CBr_4	78
Carbon tetraiodide	CI_4	79
Methyl fluoride	CH_3F	80
Methyl fluoride–d_3	CD_3F	81
Methyl chloride	CH_3Cl	82
Methyl chloride–d_3	CD_3Cl	83
Methyl bromide	CH_3Br	84
Methyl bromide–d_3	CD_3Br	85
Methyl iodide	CH_3I	86
Methyl iodide–d_3	CD_3I	87
Trifluoromethane	CHF_3	88
Trifluoromethane–d	CDF_3	320
Trichloromethane	$CHCl_3$	89
Trichloromethane–d_1	$CDCl_3$	90
Tribromomethane	$CHBr_3$	91
Tribromomethane–d_1	$CDBr_3$	92
Bromotrichloromethane	$CBrCl_3$	93
Tribromochloromethane	CBr_3Cl	94
Dichloromethane	CH_2Cl_2	95
Dichloromethane–d_1	$CHDCl_2$	96
Dichloromethane–d_2	CD_2Cl_2	97
Dibromomethane	CH_2Br_2	98
Dibromomethane–d_1	$CHDBr_2$	99
Dibromomethane–d_2	CD_2Br_2	100
Dibromodichloromethane	CBr_2Cl_2	101

Bromochloromethane	CH_2BrCl	102
Bromochloromethane-d_1	$CHDBrCl$	103
Bromochloromethane-d_2	CD_2BrCl	104
Formic acid	$HCOOH$	105
Formic acid-d_2	$DCOOD$	106

C_1-six-atomic molecules

Borine carbonyl	$^{10}BH_3CO$	321
Borine carbonyl-d_3	$^{10}BD_3CO$	322
Borine carbonyl	$^{11}BH_3CO$	323
Borine carbonyl-d_3	$^{11}BD_3CO$	324
Methanol	CH_3OH (Gas)	107
Methanol	CH_3OH (Liquid)	108
Methanol-d_1	CH_3OD (Gas)	109
Methanol-d_1	CH_3OD (Liquid)	110
Methanol-d_3	CD_3OH (Gas)	111
Methanol-d_3	CD_3OH (Liquid)	112
Methanol-d_4	CD_3OD (Gas)	113

C_1-seven-atomic molecules

Methylamine	CH_3NH_2	114
Methylamine-d_2	CH_3ND_2	115
Methylamine-d_3	CD_3NH_2	116
Methylamine-d_5	CD_3ND_2	117

C_1-eight-atomic molecules

Methylsilane	CH_3SiH_3	275
Methylsilane-d_3	CH_3SiD_3	276
Methylgermane	CH_3GeH_3	277
Methyl-d_3-germane	CD_3GeH_3	278

C_2-four-atomic molecules

Acetylene	C_2H_2	118
Acetylene-d_1	C_2HD	119
Acetylene-d_2	C_2D_2	120
Cyanogen	C_2N_2	279
Dichloroacetylene	C_2Cl_2	325
Dibromoacetylene	C_2Br_2	326
Diiodoacetylene	C_2I_2	327
Fluoroacetylene	$CHCF$	121
Chloroacetylene	$CHCCl$	122
Bromoacetylene	$CHCBr$	123
Bromochloroacetylene	C_2ClBr	328
Chloroiodoacetylene	C_2ClI	329

C_2-six-atomic molecules

Methyl cyanide	CH_3CN	143
Methyl cyanide-d_3	CD_3CN	144
Methyl isocyanide	CH_3NC	145
Methyl isocyanide-d_3	CD_3NC	146
Ethylene	C_2H_4	124
Ethylene-d_4	C_2D_4	125
Tetrafluoroethylene	CF_2CF_2	126
Tetrachloroethylene	CCl_2CCl_2	127
Tetrabromoethylene	CBr_2CBr_2	128
Trans-1,2-Difluoroethylene	$CHFCHF$	330
Trans-1,2-Difluoroethylene-d_1	$CHFCDF$	331
Trans-1,2-Difluoroethylene-d_2	$CDFCDF$	332
Trans-1,2-Dichloroethylene	$CHClCHCl$	132
Trans-1,2-Dichloroethylene-d_1	$CHClCDCl$	133
Trans-1,2-Dichloroethylene-d_2	$CDClCDCl$	134
Trans-1,2-Dichloro-1,2-Difluoroethylene	$CFClCFCl$	138
Cis-1,2-Difluoroethylene	$CHFCHF$	129
Cis-1,2-Difluoroethylene-d_1	$CHFCDF$	130
Cis-1,2-Difluoroethylene-d_2	$CDFCDF$	131
Cis-1,2-Dichloroethylene	$CHClCHCl$	135
Cis-1,2-Dichloroethylene-d_1	$CHClCDCl$	136
Cis-1,2-Dichloroethylene-d_2	$CDClCDCl$	137
1,1-Dichloroethylene	CH_2CCl_2	139
1,1-Dichloroethylene-d_1	$CHDCCl_2$	140
1,1-Dichloroethylene-d_2	CD_2CCl_2	141
1,1-Dichloro-2,2-Difluoroethylene	CF_2CCl_2	142

C_2-seven-atomic molecules

Silylacetylene	SiH_3CCH	148
Ethylene oxide	C_2H_4O	149
Ethylene oxide-d_4	C_2D_4O	150
1,2,5-Oxadiazole	$C_2H_2N_2O$	147
Acetaldehyde	CH_3CHO	151
Acetaldehyde-d_1	CH_3CDO	152
Acetaldehyde-d_4	CD_3CDO	153

C_2-eight-atomic molecules

Ethane	CH_3CH_3	154
Ethane-d_3	CH_3CD_3	155
Ethane-d_6	CD_3CD_3	156
Hexafluoroethane	CF_3CF_3	157
Hexachloroethane	CCl_3CCl_3	158
Hexabromoethane	CBr_3CBr_3	159
1,2-Dichloroethane, trans form	CH_2ClCH_2Cl	160
1,2-Dichloroethane, gauche form	CH_2ClCH_2Cl	161
1,2-Dibromoethane, trans form	CH_2BrCH_2Br	162
1,2-Dibromoethane, gauche form	CH_2BrCH_2Br	163
1-Bromo-2-chloroethane, trans form	CH_2ClCH_2Br	164
1-Bromo-2-chloroethane, trans form	CH_2ClCH_2Br	165
Fluoroethane	CH_3CH_2F	166
Chloroethane	CH_3CH_2Cl	167
Bromoethane	CH_3CH_2Br	168
Ethylene imine	C_2H_5N	169
Methyl formate	$HCOOCH_3$	170
Methyl formate-d_1	$DCOOCH_3$	171
Methyl formate-d_3	$HCOOCD_3$	172
Methyl formate-d_4	$DCOOCD_3$	173
Acetic acid	CH_3COOH	174
Acetic acid-d_1	CH_3COOD	175

C_2–nine–atomic molecules

Dimethylether	CH_3OCH_3	176
Dimethylether–d$_3$	CH_3OCD_3	177

C_3–five–atomic molecules

Carbon suboxide	C_3O_2	280
Carbon subsulfide	C_3S_2	281

C_3–seven–atomic molecules

Allene	CH_2CCH_2	178
Methylacetylene	CH_3CCH	179
Methylacetylene–d$_1$	CH_3CCD	180
Methylacetylene–d$_3$	CD_3CCH	181
Methylacetylene–d$_4$	CD_3CCD	182
Malononitrile	$NCCH_2CN$	183
Malononitrile–d$_2$	$NCCD_2CN$	184

C_3–eight–atomic molecules

Propenal	C_3H_4O	185

C_3–nine–atomic molecules

Cyclopropane	C_3H_6	186
Cyclopropane–d$_6$	C_3D_6	187
Ethylcyanide	CH_3CH_2CN	188

C_3–ten–atomic molecules

Acetone	CH_3COCH_3	189
Acetone–d$_3$	CH_3COCD_3	190
Acetone–d$_6$	CD_3COCD_3	191

C_3–eleven–atomic molecules

Propane	$CH_3CH_2CH_3$	192
Propane–d$_2$	$CH_3CD_2CH_3$	193
Propane–d$_3$	$CH_3CH_2CD_3$	194
Propane–d$_6$	$CD_3CH_2CD_3$	195
Propane–d$_8$	$CD_3CD_2CD_3$	196
Methyl acetate	CH_3COOCH_3	197
Methyl acetate–d$_3$	CD_3COOCH_3	198
Methyl–d$_3$–acetate	CH_3COOCD_3	199
Methyl acetate–d$_6$	CD_3COOCD_3	200

C_4–six–atomic molecules

Butadiyne	$HCCCCH$	201

C_4–nine–atomic molecules

Furan	C_4H_4O	202
Thiophene	C_4H_4S	203
Thiophene–d$_4$	C_4D_4S	204

C_4–ten–atomic molecules

1,3–Butadiene	$CH_2CHCHCH_2$	205
1,3–Butadiene–d$_1$, trans	$CH_2CHCHCHD$	206
1,3–Butadiene–1,1,2–d$_3$	$CH_2CHCDCD_2$	207
1,3–Butadiene–1,1,4,4–d$_4$	$CD_2CHCHCD_2$	208
1,3–Butadiene–d$_6$	$CD_2CDCDCD_2$	209
2–Butyne	CH_3CCCH_3	210

C_4–12–atomic molecules

Cyclobutane	C_4H_8	211
Cyclobutane–d$_8$	C_4D_8	212
2–Methylpropene	$(CH_3)_2CCH_2$	213
2–Methyl–d$_3$–propene–3,3,3–d$_3$	CD_3CCH_2	214

C_4–13–atomic molecules

2–Butanone, trans form	$CH_3COCH_2CH_3$	215

C_4–14–atomic molecules

1,4–Dioxane	$C_4H_8O_2$	333
n–Butane, trans form	$CH_3CH_2CH_2CH_3$	216
n–Butane, gauche form	$CH_3CH_2CH_2CH_3$	217

C_6–12–atomic molecules

Benzene	C_6H_6	218
Benzene–d$_6$	C_6D_6	219

C_6–13–atomic molecules

Hexacarbonylchromium	$Cr(^{12}C^{16}O)_6$	334
Hexacarbonylmolybdenum	$Mo(^{12}C^{16}O)_6$	335
Hexacarbonyltungsten	$W(^{12}C^{16}O)_6$	336

C_6–18–atomic molecules

Cyclohexane	C_6H_{12}	220
Cyclohexane–d$_{12}$	C_6D_{12}	221

Polymer

Poly–(methylene)	$-(CH_2)n-$	222
Poly–(methylene–d$_2$)	$-(CD_2)n-$	223

B. Empirical Formula Index

In this index molecules are divided into two groups: (a) those containing no carbon atoms, for which the formulas are arranged with the elemental symbols in alphabetical order and are listed alphabetically, and in ascending order of the empirical formula subscripts; (b) molecules containing carbon, which are ordered in the same way except that carbon is listed first and hydrogen second. No distinction is made for isotopic species in the empirical formula; thus deuterium is listed as H.

Compounds Not Containing Carbon

AsF_3	Arsenic trifluoride	292
AsF_5	Arsenic pentafluoride	306
AsH_3	Arsine	21
AsH_3	Arsine–d_3	22
BF_3	Boron trifluoride–$^{10}BF_3$	238
BF_3	Boron trifluoride–$^{11}BF_3$	239
B_2H_6	Diborane–$^{11}B_2H_6$	55
B_2H_6	Diborane–$^{10}B_2D_6$	56
$BrCl_3Si$	Bromotrichlorosilane	45
BrF_3	Bromine trifluoride	290
$BrGeH_3$	Germyl bromide	263
$BrGeH_3$	Germyl bromide–d_3	264
BrH_3Si	Silyl bromide	44
$BrNO$	Nitrosyl bromide–$^{16}O^{14}NBr$	235
$BrNO$	Nitrosyl bromide–$^{16}O^{15}NBr$	236
$BrNO$	Nitrosyl bromide–$^{18}O^{15}NBr$	237
Br_2Cl_2Si	Dibromodichlorosilane	49
Br_2FOP	Phosphoryl fluorodibromide	303
Br_2H_2Si	Dibromosilane	301
Br_2OS	Thionyl bromide	250
Br_3ClSi	Tribromochlorosilane	47
Br_3GeH	Tribromogermane	268
Br_3HSi	Tribromosilane	255
Br_3OP	Phosphoryl bromide	258
Br_4Ge	Germanium tetrabromide	39
Br_4Si	Silicon tetrabromide	31
Br_4Sn	Tin (IV) bromide	41
ClF_3	Chlorine trifluoride	289
ClF_5S	Sulfur chloride pentafluoride	308
ClF_5W	Tungsten chloride pentafluoride	309
$ClGeH_3$	Germyl chloride	261
$ClGeH_3$–d_3	Germyl chloride–d_3	262
$ClHO$	Hypochlorous acid	284
$ClHO$	Hypochlorous acid–d	2855
ClH_3Si	Silyl chloride	43
ClI_3Si	Chlorotriiodosilane	48
$ClNO$	Nitrosyl chloride–$^{16}O^{14}NO$	231
$ClNO$	Nitrosyl chloride–$^{16}O^{15}NCl$	232
$ClNO$	Nitrosyl chloride–$^{18}O^{14}NCl$	233
$ClNO$	Nitrosyl chloride–$^{18}O^{15}NCl$	234
$ClNO_2$	Nitryl chloride–$Cl^{14}NO_2$	235
$ClNO_2$	Nitryl chloride–$Cl^{15}NO_2$	244
$ClNS$	Thionitrosyl–S–chloride	287
Cl_2FOP	Phosphoryl fluorodichloride	302
Cl_2H_2Si	Dichlorosilane	299
Cl_2H_2Si	Dichlorosilane–d_2	300
Cl_2O	Oxygen dichloride	8
Cl_2OS	Thionyl chloride	249
Cl_2O_2S	Sulfuryl chloride	270
Cl_2S	Sulfur dichloride	226
Cl_3GeH	Trichlorogermane	267
Cl_3HSi	Trichlorosilane	253
Cl_3HSi	Trichlorosilane–d	254
Cl_3ISi	Trichloroiodosilane	46
Cl_3OP	Phosphoryl chloride	257
Cl_3P	Phosphorus trichloride	20
Cl_4Ge	Germanium tetrachloride	38
Cl_4Si	Silicon tetrachloride	30
Cl_4Sn	Tin (IV) chloride	40
$FGeH_3$	Germyl fluoride	259
$FGeH_3$	Germyl fluoride–d_3	260
FH_3Si	Silyl fluoride	42
FNO	Nitrosyl fluoride–$^{16}O^{14}NF$	227
FNO	Nitrosyl fluoride–$^{16}O^{15}NF$	228
FNO	Nitrosyl fluoride–$^{18}O^{14}NF$	229
FNO	Nitrosyl fluoride–$^{18}O^{15}NF$	230
FNO_2	Nitryl fluoride–$F^{14}NO_2$	241
FNO_2	Nitryl fluoride–$F^{15}NO_2$	242
FNS	Thionitrosyl–S–fluoride	286
F_2HN	Difluoroamine	295
F_2N_2	Trans–1,2–Difluorodiazine	288
F_2	Oxygen difluoride	7
F_2OS	Thionyl fluoride	248
F_2O_2S	Sulfuryl fluoride	269
F_2O_2Se	Selenium dioxide difluoride	271
F_2S_2	Difluoro disulfane	294
F_3HSi	Trifluorosilane	251
F_3HSi	Trifluorosilane–d	252
F_3N	Nitrogen trifluoride	16
F_3OP	Phosphoryl fluoride	256
F_3P	Phosphorus trifluoride	19
F_4Si	Silicon tetrafluoride	29
F_5	Phosphorus pentafluoride	304
F_5V	Vanadium pentafluoride	305
F_6Ir	Iridium fluoride	307
F_6Mo	Molybdenum (IV) fluoride	52
F_6S	Sulfur hexafluoride	50
F_6Se	Selenium hexafluoride	51
F_6Te	Tellurium hexafluoride	272
F_6U	Uranium (IV) fluoride	54
F_6W	Tungsten (IV) fluoride	53
GeH_3I	Germyl iodide	265
GeH_3I	Germyl iodide–d_3	266
GeH_4	Germane	33
GeH_4	Germane–d_1	34
GeH_4	Germane–d_2	35
GeH_4	Germane–d_3	36
GeH_4	Germane–d_4	37
Ge_2H_6	Digermane	273
Ge_2H_6	Digermane–d_6	274
HN_3	Hydrazoic acid	245
HN_3	Hydrazoic acid–d_1	246
H_2O	Water	4
H_2O	Water–$H_2{}^{18}O$	282
H_2O	Water–d_1	5
H_2O	Water–d_2	6
H_2O_2	Hydrogen peroxide	247
H_2S	Hydrogen sulfide	9
H_2S	Deuterium sulfide	10
H_2S_2	Hydrogen persulfide	293
H_2Se	Hydrogen selenide	12
H_2Se	Hydrogen deuterium selenide	13
H_3N	Ammonia	14
H_3N	Ammonia–d_3	15
H_3N	Ammonia–t_3	291

H_3P	Phosphine	17
H_3P	Phosphine-d_3	18
H_3Sb	Stibine	23
H_3Sb	Stibine-d_3	24
H_4Si	Silane	25
H_4Si	Silane-d_2	26
H_4Si	Silane-d_3	27
H_4Si	Silane-d_4	28
I_4Si	Silicon tetraiodide	32
NO_2	Nitrogen dioxide-$^{14}NO_2$	224
NO_2	Nitrogen dioxide-$^{15}NO_2$	225
N_2O	Nitrous oxide	1
N_2O	Nitrous oxide-$^{14}N^{15}NO$	2
N_2O	Nitrous oxide-$^{15}N_2O$	3
O_2S	Sulfur dioxide	11
O_2S	Sulfur dioxide-$S^{18}O_2$	283
O_3S	Sulfur trioxide	240
O_4Os	Osmium tetroxide-$Os^{16}O_4$	297
O_4Os	Osmium tetroxide-$Os^{18}O_4$	298
O_4Ru	Ruthenium tetroxide	296

Compounds Containing Carbon

CBrClO	Carbonyl bromochloride	319
$CBrCl_3$	Bromotrichloromethane	93
CBrN	Cyanogen bromide-$^{79}BrCN$	66
CBrN	Cyanogen bromide-$^{81}BrCN$	67
CBr_2Cl_2	Dibromodichloromethane	101
CBr_2O	Carbonyl bromide	314
CBr_3Cl	Tribromochloromethane	94
CBr_4	Carbon tetrabromide	78
CClFO	Carbonyl chlorofluoride	318
CClN	Cyanogen chloride-$^{35}ClCN$	64
CClN	Cyanogen chloride-$^{37}ClCN$	65
CCl_2O	Carbonyl chloride	313
CCl_4	Carbon tetrachloride	77
CFN	Cyanogen fluoride	310
CF_2O	Carbonyl fluoride	312
CF_2S	Thiocarbonyl fluoride	315
CF_4	Carbon tetrafluoride	76
CIN	Cyanogen iodide	311
CI_4	Carbon tetraiodide	79
COS	Carbonyl sulfide	61
CO_2	Carbon dioxide	58
CO_2	Carbon dioxide-$^{13}CO_2$	59
CS_2	Carbon disulfide	60
$CHBr_3$	Tribromomethane	91
$CHBr_3$	Tribromomethane-d_1	92
$CHCl_3$	Trichloromethane	89
$CHCl_3$	Trichloromethane-d_1	90
CHF_3	Trifluoromethane	88
CHF_3	Trifluoromethane-d	320
CHN	Hydrogen cyanide	62
CHN	Deuterium cyanide	63
CHNO	Isocyanic acid	316
CHNO	Isocyanic acid-d	317
CH_2BrCl	Bromochloromethane	102
CH_2BrCl	Bromochloromethane-d_1	103
CH_2BrCl	Bromochloromethane-d_2	104
CH_2Br_2	Dibromomethane	98
CH_2Br_2	Dibromomethane-d_1	99
CH_2Br_2	Dibromomethane-d_2	100
CH_2Cl_2	Dichloromethane	95
CH_2Cl_2	Dichloromethane-d_1	96
CH_2Cl_2	Dichloromethane-d_2	97
CH_2O	Formaldehyde	68
CH_2O	Formaldehyde-d_1	69
CH_2O	Formaldehyde-d_2	70
CH_2O_2	Formic acid	105
CH_2O_2	Formic acid-d_2	106
CH_3BO	Borine carbonyl-$^{10}BH_3CO$	321
CH_3BO	Borine carbonyl-d_3 $^{10}BD_3CO$	322
CH_3BO	Borine carbonyl-$^{11}BH_3CO$	323
CH_3BO	Borine carbonyl-$d_3$$^{11}BD_3CO$	324
CH_3Br	Methyl bromide	84
CH_3Br	Methyl bromide-d_3	85
CH_3Cl	Methyl chloride	82
CH_3Cl	Methyl chloride-d_3	83
CH_3F	Methyl fluoride	80
CH_3F	Methyl fluoride-d_3	81
CH_3I	Methyl iodide	86
CH_3I	Methyl iodide-d_3	87
CH_4	Methane	71
CH_4	Methane-d_1	72
CH_4	Methane-d_2	73
CH_4	Methane-d_3	74
CH_4	Methane-d_4	75
CH_4O (Gas)	Methanol	107
CH_4O (Liquid)	Methanol	108
CH_4O (Gas)	Methanol-d_1	109
CH_4O (Liquid)	Methanol-d_1	110
CH_4O (Gas)	Methanol-d_3	111
CH_4O (Liquid)	Methanol-d_3	112
CH_4O (Gas)	Methanol-d_4	113
CH_5N	Methylamine	114
CH_5N	Methylamine-d_2	115
CH_5N	Methylamine-d_3	116
CH_5N	Methylamine-d_5	117
CH_6Ge	Methylgermane	277
CH_6Ge	Methyl-d_3-germane	278
CH_6Si	Methylsilane	275
CH_6Si	Methylsilane-d_3	276
C_2BrCl	Bromochloroacetylene	328
C_2Br_2	Dibromoacetylene	326
C_2Br_4	Tetrabromoethylene	128
C_2Br_6	Hexabromoethane	159
C_2ClI	Chloroiodoacetylene	329
C_2Cl_2	Dichloroacetylene	325
$C_2Cl_2F_2$	trans-1,2-Dichloro-1,2-diflurorethylene	138
$C_2Cl_2F_2$	1,1-Dichloro-2,2-difluoroethylene	142
C_2Cl_4	Tetrachloroethylene	127
C_2Cl_6	Hexachloroethane	158
C_2F_4	Tetrafluoroethylene	126
C_2F_6	Hexafluoroethane	157